PRICM 11 The 11th Pacific Rim International Conference on Advanced Materials and Processing

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# PRICM 11

## The 11th Pacific Rim International Conference on Advanced Materials and Processing

**November 19-23, 2023** | ICC, Jeju, Korea



**Hosted by**

The Korean Institute of Metals and Materials

**Co-Hosted by**

Materials Australia

The Japan Institute of Metals and Materials

The Minerals, Metals & Materials Society

The Chinese Society for Metals

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# AMAZEMET®

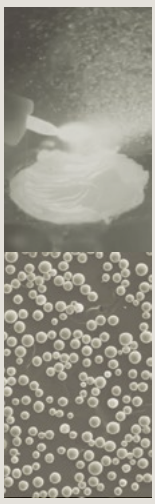
AMAZEMET is a spin-off company of the Warsaw University of Technology. The company was created as a result of challenges faced by its founder during his research on BMG 3D printing, when it turned out that solutions created in the process might help also other researchers. Offered products aim to create new possibilities in materials development, especially metallic powders and metal additive manufacturing.
AMAZEMET maintains a strong connection with academic researchers by participating in collaborative research activities focused on developing new materials for 3D printing and partnering in projects, such as:

- EIC Pathfinder
- Horizon 2020
- M-ERA.net
- ESA.

## | rePOWDER |

**Ultrasonic powder atomizer and alloy prototyping platform**

- Ultrasonic atomizer with arc melter functionality and induction furnace.
- Processing of any alloy composition from any feedstock - pure elements, rod, wire, failed printouts and more.






## | inFURNER |

**Compact high vacuum furnace**

- Laboratory-size, compatible with popular LPBF printers.
- Temperatures up to 1200°C or 1600°C and vacuum up to $3x10^{-7}$ mbar.
- Custom treatment programs with quenching options available.





| AM |

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This work was supported by the Korean Federation of Science and Technology Societies( KOFST) grant funded by the Korean government.

# **Welcome** Message



## Hyoung Seop Kim

Organizing Chair of PRICM11
Chair Professor, POSTECH

On behalf of the organizing committee, it is our great pleasure to cordially invite you to the 11th Pacific Rim International Conference on Advanced Materials and Processing (PRICM11). For more than 30 years, PRICM has served as an international stage for dissemination of current and emerging materials and processing, jointly organized by the Chinese Society for Metals (CSM), The Japan Institute of Metals and Materials (JIM), The Korean Institute of Metals and Materials (KIM), Materials Australia (MA), and The Minerals, Metals & Materials Society (TMS).

In 2023, PRICM11 will be held as an onsite event from November 19-23 at the INTERNATIONAL CONVENTION CENTER in Jeju island, Korea. The Conference will definitely provide an attractive forum for presenting the most recent advances in advanced materials and processing by researchers and engineers from industry, research laboratories, and academia. The Plenary, Keynote, Invited and Contributed presentations will be included. All the presentations from leading-edge academia and industrial research settings in related areas will provide a lucid and comprehensive overview of the current status and potential future directions for materials research and development.

I look forward to your contribution and participation.

Hyoung Seop Kim

# Committees / Organizers

### Conference Chair

Hyoung Seop Kim (Pohang University of Science and Technology, Korea)

### Honorary Chair

Sung-Joon Kim (Pohang University of Science and Technology, Korea)

### Secretary General

Jae Bok Seol (Gyeongsang National University, Korea)

## Local Organizing Committee (KIM)

Hyoung Seop Kim (Pohang University of Science and Technology)
Jae Bok Seol (Gyeongsang National University)
Hyun Joo Choi (Kookmin University)
Kisub Cho (Kookmin University)
Seok Su Sohn (Korea University)
Ho Jin Ryu (Korea Advanced Institute of Science and Technology)
Kee Ahn Lee (Inha University)
Young Sang Na (Korea Institute of Materials Science)
Junhee Han (Korea Institute of Industrial Technology)
Won-Seok Ko (Inha University)
Jae Wung Bae (Pukyong National University)
Bin Lee (Kyung Hee University)

## In-Country Representative

**KIM** Hyoung Seop Kim (Pohang University of Science and Technology)
**MA** Jian-Feng Nie (Monash University)
**TMS** George (Rusty) Gray (Los Alamos National Laboratory)
**JIMM** Yoshihito KAWAMURA (Kumamoto University)
**CSM** Chengjia Shang (University of Science & Technology Beijing)

## International Organizing Committee

**KIM** Young Keun Kim (Korea University)
Heung Nam Han (Seoul National University)
Il Sohn (Yonsei University)
**MA** Sophie Primig (University of New South Wales)
Daniel East (CSIRO Manufacturing)
Gwénaëlle Proust (The University of Sydney)
**TMS** Nikhilesh Chawla (Purdue University)
Saryu Fensin (Los Alamos National Laboratory)
Paul Ohhodnicki (University of Pittsburgh)
**JIMM** Hideyuki Yasuda (Kyoto University)
Manabu Enoki (The University of Tokyo)
Takayoshi Nakano (Osaka University)
**CSM** Chengjia Shang (University of Science &Technology Beijing)
ZhilingTian (Chinese Society for Metals)
Guoqing Zhang (Beijing Institute of Aeronautical Materials)

## International Advisory Board Members

**KIM** Sung-Joon Kim (Pohang University of Science and Technology)
Hyuck Mo Lee (Korea Advanced Institute of Science and Technology)
Je-Hyun Lee (Changwon National University)
**MA** Ivan Cole (RMIT University)
Nikki Stanford (University of South Australia)
Allan Morton (Monash University)
**TMS** Elizabeth A. Holm (Carnegie Mellon University)
W. Jud Ready (Georgia Institute of Technology)
Dan J. Thoma (University of Wisconsin-Madison)

# Committees / Organizers

**JIMM** Satoshi Sugimoto (Tohoku University)
Haruyuki Inui (Kyoto University)
Koki Takanashi (Japan Atomic Energy Agency/ Tohoku University)

**CSM** Bingbo Wei (Northwestern Polytechnical University)
Huibin Xu (Beihang University)
Yue Zhang (University of Science &Technology Beijing)

## Symposium Organizers

### Symposium A. Advanced Steels and Properties

**KIM**
Byoungchul Hwang (Seoul National University of Science and Technology)
Seok Su Sohn (Korea University)
Jeongho Han (Hanyang University)

**MA**
Sophie Primig (The University of New South Wales)

**JIMM**
Takahito OMURA (NIMS)
Yoshikazu TODAKA (Toyohashi University of Technology)

**CSM**
Xuejun Jin (Shanghai Jiao Tong University)
Hao Chen (Tsinghua University)

### Symposium B. Advanced Processing of Materials

**KIM**
Hwijun Kim (Korea Institute of Industrial Technology)
EUN SOO PARK (Seoul National University)

**MA**
Daniel East (CSIRO Manufacturing)

**JIMM**
Hideyuki YASUDA (Kyoto University)
Katsunari OIKAWA (Tohoku University)

**CSM**
Wei Xu (Northeastern University)
Qiaodan Hu (Shanghai Jiaotong University)

### Symposium C. Structural Materials for High Temperature

**KIM**
Sung-Soo RYU (Korea Institute of Ceramic Engineering and Technology)
Jongmin Byun (Seoul National University of Science and Technology)

**MA**
Matthew Dargusch (The University of Queensland)

**JIMM**
Hiroyuki YASUDA (Osaka University)
Kyosuke YOSHIMI (Tohoku University)

**CSM**
Qiang Feng (University of Science and Technology Beijing)
Zhongnan Bi (Central Iron & Steel Research Institute)
Yunsong Zhao (AECC Bejing Institute of Aeronautical Materials)

### Symposium D. Light Metals and Alloys

**KIM**
Hyun Joo Choi (Kookmin University)
Young Min Kim (Korea Institute of Materials Science)

**MA**
Jian-Feng Nie (Monash University)

**JIMM**
Yoshihito KAWAMURA (Kumamoto University)
Yoko MITARAI (University of Tokyo)
Shoichi HIROSAWA (Yokohama National University)

**CSM**
Yongqing Zhao (Northwest Institute for Nonferrous Metal Research)
Xianhua Chen (Chongqing University)

# Committees / Organizers

## Symposium E. Additive Manufacturing

**KIM**

Ji-Hun YU (Korea Institute of Materials Science)
Bin Lee (Kyung Hee University)
Junhee Han (Korea Institute of Industrial Technology)

**MA**

Ma Qian (RMIT University)

**JIMM**

Takayoshi NAKANO (Osaka University)
Yuichiro KOIZUMI (Osaka University)

**CSM**

Shaoming Zhang (China Iron & Steel Research Institute Group)
Xuanhui Qu (University of Science and Technology Beijing)

## Symposium F. Thin Films and Surface Engineering

**KIM**

Ho Won Jang (Seoul National University)
Soo Young Kim (Korea University)

**MA**

Chris Berndt (Swinburne University of Technology)

**JIMM**

Hiroshi MASUMOTO (Tohoku University)
Shigenari HAYASHI (Hokaido University)

**CSM**

Chuang Dong (Dalian University of Technology)
Hongbo Guo (Beihang University)

## Symposium G. Materials for Energy Storage and Generation

**KIM**

Dong-Hwa Seo (Korea Advanced Institute of Science and Technology)
IL JEON (Sungkyunkwan University)
Yeongbeom Cheon (Korea Atomic Energy Research Institute)

**JIMM**

Tetsuya UDA (Kyoto University)
Naoyuki HASHIMOTO (Hokaido University)

**CSM**

Ming Zhu (South China University of Technology)
Guang-Hong Lu (Beihang University)

## Symposium H. Electronic and Magnetic Materials

**KIM**

Wooyoung Lee (Yonsei University)
Haein Yim (Sookmyung Women's University)

**MA**

Lan Fu (The Australian National University)

**JIMM**

Yuu SHIRATUCHI (Osaka University)
Seishi ABE (Research Institute for Electromagnetic Materials)

**CSM**

Chengbao Jiang (Beihang University)
Shouguo Wang (Anhui University)

## Symposium I. Biomaterials and Soft Materials and their Application

**KIM**

Hyun Kwang Seok (Korea Institute of Science and Technology)
Jongtaek Yeom (Korea Institute of Materials Science)

**MA**

Tim Hughes (CSIRO Manufacturing)

**JIMM**

Yusuke TSUTSUMI (NIMS)
Masaya YAMAMOTO (Tohoku University)

**CSM**

Yufeng Zheng (Peking University)
Luning Wang (University of Science and Technology Beijing)

## Symposium J. Materials Characterization and in situ/3D/4D Analysis

**KIM**

Dong-Ik Kim (Korea Institute of Science and Technology)
Jae Bok Seol (Gyeongsang National University)

# Committees / Organizers

**MA**
Gwenaelle Proust (The University of Sydney)
**JIMM**
Naoya SHIBATA (University of Tokyo)
Satoshi HATA (Kyushu University)
**CSM**
Zhiwei Shan (Xi'an Jiaotong University)
Xiaodong Han (Beijing University of Technology)

## Symposium K. High-Entropy Materials and Amorphous Materials

**KIM**
Ho Jin Ryu (Korea Advanced Institute of Science and Technology)
Young Sang Na (Korea Institute of Materials Science)
Ki Buem Kim (Sejong University)
**MA**
Kevin Laws (The University of New South Wales)
**JIMM**
Hariyuki INUI (Kyoto University)
Hidemi KATO (Tohoku University)
**CSM**
Zhaoping Lu (University of Science and Technology Beijing)
Kefu Yao (Tsinghua University)
Yiping Lu (Dalian University of Technology)

## Symposium L. Composite, Coating and Hetero-Materials

**KIM**
Sang-Bok Lee (Korea Institute of Materials Science)
Caroline Sunyong Lee (Hanyang University)
**MA**
Chun Hui Wang (The University of New South Wales)
**JIMM**
Hideki HOSODA (Tokyo Institute of Technology)
Yoshimi WATANABE (Nagoya Institute of Technology)
**CSM**
Di Zhang (Shanghai Jiaotong University)
Lin Geng (Harbin Institute of Technology)
Huaxin Peng (Zhejiang University)

## Symposium M. Nano Materials and Nano Severe Plastic Deformation

**KIM**
Yoon Suk Choi (Pusan National University)
Dong-Hyun Lee (Chungnam National University)
**MA**
Yuri Estrin (Monash University)
**JIMM**
Nobuhiro TSUJI (Kyoto University)
Masaki TANAKA (Kyushu University)
**CSM**
Qingliang Liao (University of Science and Technology Beijing)
Xiaoxu Huang (Chongqing University)
Zhuo Kang (University of Science and Technology Beijing)

## Symposium N. Computational Materials and Artificial Intelligence

**KIM**
Pil-Ryung Cha (Kookmin University)
Won-Seok Ko (Inha University)
Kisub Cho (Kookmin University)
**MA**
Bernard Rolfe (Deakin University)
**JIMM**
Junya INOUE (University of Tokyo)
Toshiyuki KOYAMA (Nagoya University)
**CSM**
Yanjing Su (University of Science and Technology Beijing)
Zhimei Sun (Beihang University)

# Committees / Organizers

### Symposium O. Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**KIM**

Taek-soo Kim (Korea Institute of Industrial Technology)

Seongmook Cho (Pukyong National University)

**MA**

Ivan Cole (RMIT University)

**JIMM**

Yoshinao KOBAYASHI (Tokyo Institute of Technology)

Manabu ENOKI (University of Tokyo)

**CSM**

Han Dong (Shanghai University)

Zhiyong Liu (Chinese Society for Corrosion and Protection)

### Symposium P. 4th KIM-CSM symposium: New Metal Materials: Low-carbon emission, New energy vehicles & Lightweights

**KIM**

Hyoung-Wook Kim (Korea Institute of Materials Science)

**CSM**

Hongzhou Lu (CITIC Metal Co.,Ltd.)

# **Conference** information

## On-site Registration Desk

Lobby, 3F, JEJU ICC

| | |
|---|---|
| November 19 (SUN.) | 15:00-18:00 |
| November 20 (MON.) | 08:00-18:00 |
| November 21 (TUE.) | 08:00-18:00 |
| November 22 (WED.) | 08:00-18:00 |
| November 23 (THUR.) | 08:00-14:00 |

## Speaker's Preview Room

#304, 3F, JEJU ICC

| | |
|---|---|
| November 20 (MON.) | 08:30-18:00 |
| November 21 (TUE.) | 08:30-18:00 |
| November 22 (WED.) | 08:30-18:00 |
| November 23 (THUR.) | 08:30-14:00 |

## Exhibition Hours

Lobby, 3F, JEJU ICC

| | |
|---|---|
| November 20 (MON.) | 10:00-18:00 |
| November 21 (TUE.) | 09:00-18:00 |
| November 22 (WED.) | 09:00-18:00 |
| November 23 (THUR.) | 09:00-12:30 |

**Exhibitor Move-in:** November 19 (Sun.) 13:00-18:00
**Exhibitor Move-out:** November 23 (Thur.) 12:30-16:00

# Sponsor & Exhibition

## Host & Co-Host

- The Korean Institute of Metals and Materials
- Materials Australia
- The Minerals, Metals & Materials Society
- The Japan Institute of Metals and Materials
- The Chinese Society for Metals

## Sponsors

### Diamond

- POSCO

### Platinum

- Korean Federation of Science and Technology Societies
- Korea Tourism Organization
- Jeju Convention & Visitors Bureau (JCVB)

### Gold

- Hanwha Aerospace

### Silver

- AMAZEMET Sp. z o. o..

## Exhibition

- NEXTRON
- Thermo-Calc Software Korea LLC
- Virtual Lab. Inc
- MTDI Co., Ltd.
- Cryo H&I. INC
- Korea Institute of Industrial Technology (KITECH)

# **Official** Social Program

Social programs are designed to provide a chance for quality relaxation and entertainment during the conference. These programs will offer a great opportunity to reestablish old friendships and create new ones with colleagues from all over the world.

※ Details on social programs are subject to change according to the circumstances of the organizer.

## 1 Welcome Reception

**Date & Time:** November 19 (Sun.) 17:30-19:00

**Place:** 5F Ocean View

## 2 Poster Sessions with Refreshments

**Date & Time :** November 20 (Mon.) 18:00-19:30,
November 22 (Wed.) 18:00-19:30

**Place:** 3F Lobby

## 3 Banquet

**Date & Time :** November 21 (Tue.) 18:30-20:30

**Place :** 5F Tamna Hall B+C

## 4 Pre-conference tour

**Date and Time :** November 19 (Sun.) 09:00-14:00

**Itinerary :** ICC - Saeyeongyo Bridge - Cheonjiyeon Falls – Lunch-ICC

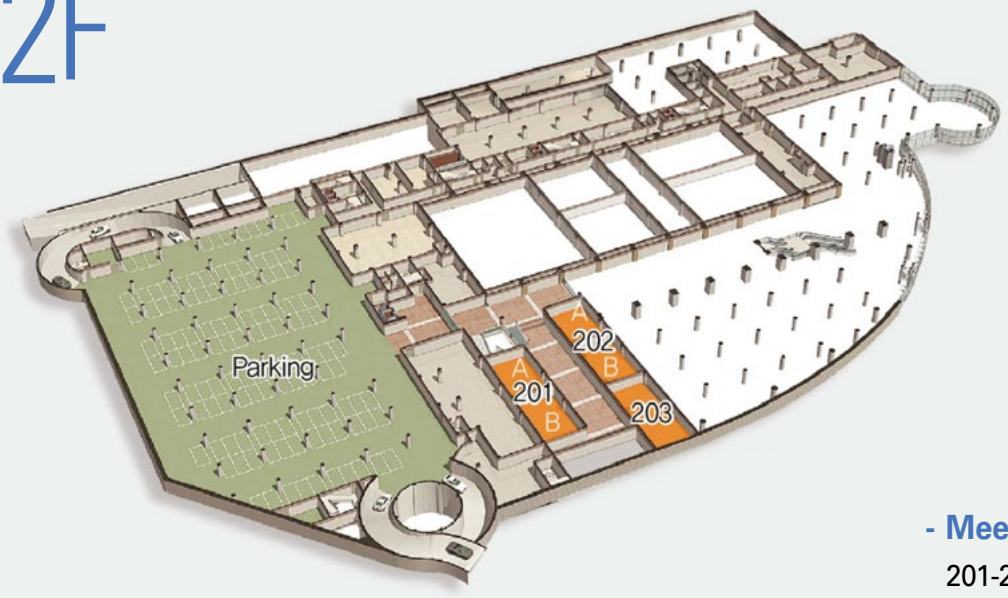
## 5 Post-conference tour

**Date and Time :** November 24 (Fri.) 09:00-16:00

**Itinerary :** ICC - Jeju Gotjawal Provincial Park - Foot Bath Therapy -Lunch - Sinchang Windmill Coastal Road - Sanbangsan Mountain - ICC

# **Floor** Plan

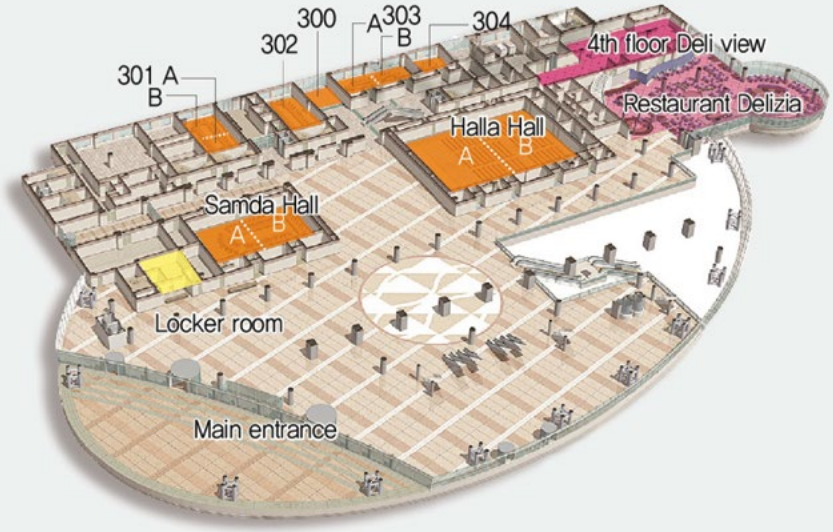
## 2F




**- Meeting Room**

201-203

## 3F




**- Lobby**

Registration Desk
Poster Presentation
Exhibition Booth

**- Meeting Room**

301-304
Samda Hall
Halla Hall

**- #302**

Comm. Lounge

**- #304**

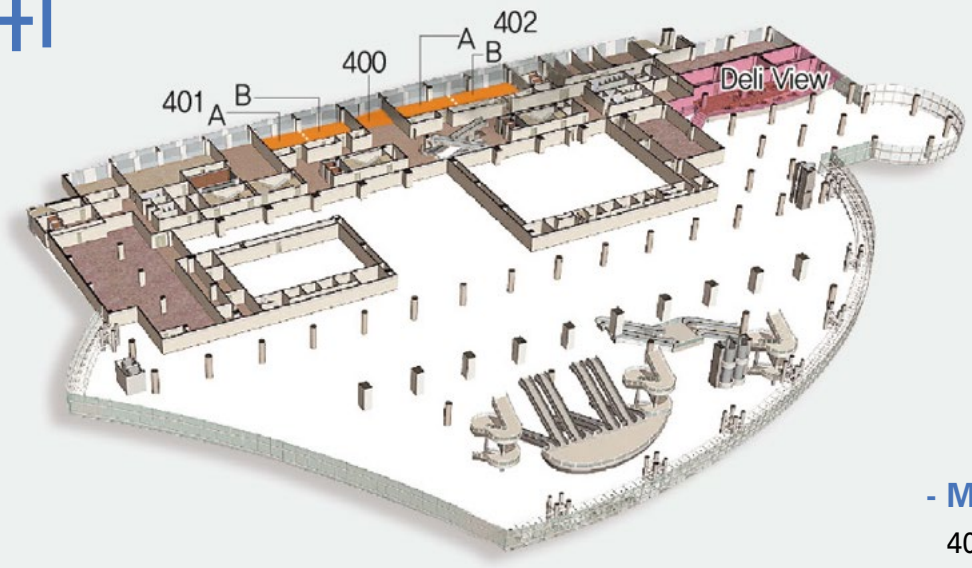
Speaker's
Preview Room

**- #300**

Secretariat

# **Floor** Plan

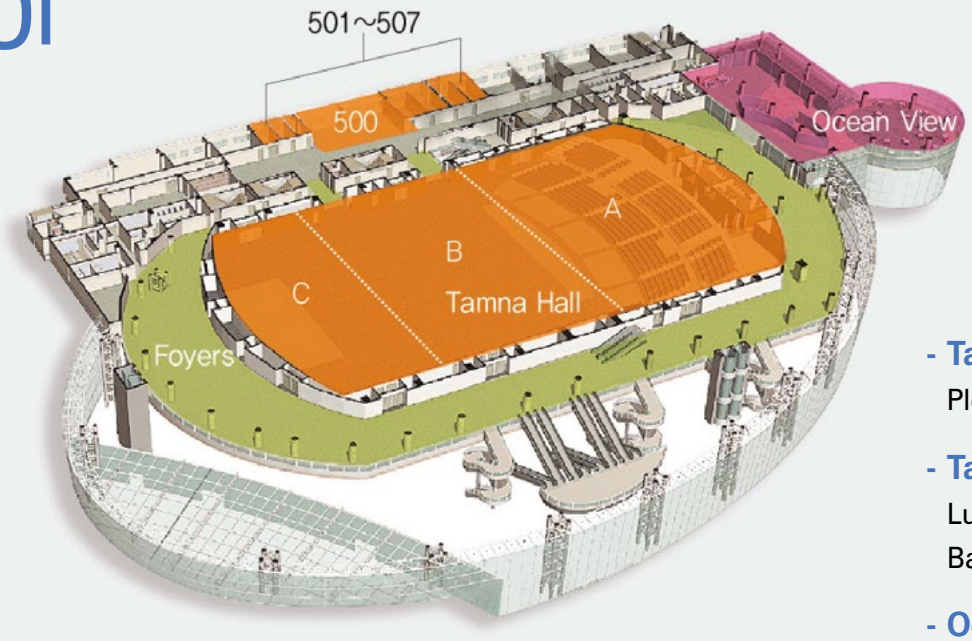
## 4F




**- Meeting Room**

400-402

## 5F




**- Tamna Hall A**

Plenary Sessions

**- Tamna Hall B+C**

Lunch

Banquet

**- Ocean View**

Welcome Reception

# **Program** at a Glance

| | Nov. 19 (Sun.) | Nov. 20 (Mon.) | Nov. 21 (Tue.) | Nov. 22 (Wed.) | Nov. 23 (Thur.) |
|---|---|---|---|---|---|
| 08:00~09:00 | | Registration (3F, Registration Desk) | | | |
| 09:00~09:40 | | Opening Ceremony | Plenary session 2<br>Dr. George T. (Rusty) Gray III<br>(Los Alamos Nat'l Lab.) | Plenary Session 4<br>Prof. Fusheng Pan<br>(Chongqing University) | Parallel Oral Session 10 |
| 09:40~10:20 | | Plenary session 1<br>Prof. Byeong-Joo Lee<br>(POSTECH) | Plenary Session 3<br>Prof. Matthew Barnett<br>(Deakin University) | Plenary Session 5<br>Prof. Tadashi Furuhara<br>(Tohoku University) | |
| 10:20~10:50 | | Coffee Break | | | |
| 10:50~12:30 | | Parallel Oral Session 1 | Parallel Oral Session 4 | Parallel Oral Session 7 | Parallel Oral Session 11 |
| 12:30~14:00 | | Lunch (5F, Tamna Hall B+C) | | | |
| 14:00~15:30 | Registration<br>(15:00~) | Parallel Oral Session 2 | Parallel Oral Session5 | Parallel Oral Session 8 | Parallel Oral Session 12 |
| 15:30~16:00 | | Coffee Break | | | Closing Ceremony |
| 16:00~18:00 | Welcome Reception<br>(17:30-19:00) | Parallel Oral Session 3 | Parallel Oral Session6 | Parallel Oral Session 9 | |
| 18:00~19:30 | | Poster Session 1 | Banquet<br>(18:30-20:30,<br>5F Tamna Hall B+C) | Poster Session 2 | |
| 19:30~20:30 | | | | | |

**Symposia**

- **A.** Advanced Steels and Properties
- **B.** Advanced Processing of Materials
- **C.** Structural Materials for High Temperature
- **D.** Light Metals and Alloys
- **E.** Additive Manufacturing
- **F.** Thin Films and Surface Engineering
- **G.** Materials for Energy Storage and Generation
- **H.** Electronic and Magnetic Materials
- **I.** Biomaterials and Soft Materials and their Application
- **J.** Materials Characterization and in situ/3D/4D Analysis
- **K.** High-Entropy Materials and Amorphous Materials
- **L.** Composite, Coating and Hetero-Materials
- **M.** Nano Materials and Nano Severe Plastic Deformation
- **N.** Computational Materials and Artificial Intelligence
- **O.** Materials for Sustainability (Green Steel, Recycling, and Corrosion)
- **P.** 4th KIM-CSM symposium: New Metal Materials: Low-carbon emission, New energy vehicles & Lightweights

# **Session** Timetable

## NOVEMBER 19 (Sunday)

| | Program |
|---|---|
| 15:00~17:30 | **Registration** |
| 17:30~19:00 | **Welcome** Reception |

## NOVEMBER 20 (Monday)

| | 201 A | 201 B | 202 A | 202 B | 203 | Halla A | Halla B |
|---|---|---|---|---|---|---|---|
| 09:20~09:40 | **Opening** Ceremony (Tamna Hall A, 5F) | | | | | | |
| 09:40~10:20 | **Plenary** Session 1<br>Prof. Byeong-Joo Lee (POSTECH, Korea) | | | | | | |
| 10:20~10:50 | Coffee Break 1 | | | | | | |
| 10:50~12:30 | **C1**<br>Structural Materials for High Temperature | **J1**<br>Materials Characterization and in situ/3D/4D Analysis | **F1**<br>Thin Films and Surface Engineering | **L1**<br>Composite, Coating and Hetero-Materials | **N1**<br>Computational Materials and Artificial Intelligence | **A1**<br>Advanced Steels and Properties | **E1**<br>Additive Manufacturing |
| 12:30~14:00 | **Lunch 1** (Tamna Hall B+C, 5F) | | | | | | |
| 14:00~15:30 | **C2**<br>Structural Materials for High Temperature | **J2**<br>Materials Characterization and in situ/3D/4D Analysis | **F2**<br>Thin Films and Surface Engineering | **L2**<br>Composite, Coating and Hetero-Materials | **N2**<br>Computational Materials and Artificial Intelligence | **A2**<br>Advanced Steels and Properties | **E2**<br>Additive Manufacturing |
| 15:30~16:00 | Coffee Break 2 | | | | | | |
| 16:00~18:00 | **C3**<br>Structural Materials for High Temperature | **J3**<br>Materials Characterization and in situ/3D/4D Analysis | **F3**<br>Thin Films and Surface Engineering | **L3**<br>Composite, Coating and Hetero-Materials | **N3**<br>Computational Materials and Artificial Intelligence | **A3**<br>Advanced Steels and Properties | **E3**<br>Additive Manufacturing |
| 18:00~19:30 | **POSTER** Session 1 | | | | | | |

# **Session** Timetable

## NOVEMBER 19 (Sunday)

| Program | |
|---|---|
| **Registration** | 15:00~17:30 |
| **Welcome** Reception | 17:30~19:00 |

## NOVEMBER 20 (Monday)

| Samda A | Samda B | 301 | 303 A | 303 B | 400 | 401 | 402 | |
|---|---|---|---|---|---|---|---|---|
| **Opening** Ceremony (Tamna Hall A, 5F) | | | | | | | | 09:20~09:40 |
| **Plenary** Session 1<br>Prof. Byeong-Joo Lee (POSTECH, Korea) | | | | | | | | 09:40~10:20 |
| Coffee Break 1 | | | | | | | | 10:20~10:50 |
| D1<br>Light Metals and Alloys | K1<br>High-Entropy Materials and Amorphous Materials | B1<br>Advanced Processing of Materials | G1<br>Materials for Energy Storage and Generation | H1<br>Electronic and Magnetic Materials | I1<br>Biomaterials and Soft Materials and their Application | O1<br>Materials for Sustainability | M1<br>Nano Materials and Nano Severe Plastic Deformation | 10:50~12:30 |
| **Lunch 1** (Tamna B+C, 5F) | | | | | | | | 12:30~14:00 |
| **D2**<br>Light Metals and Alloys | **K2**<br>High-Entropy Materials and Amorphous Materials | **B2**<br>Advanced Processing of Materials | **G2**<br>Materials for Energy Storage and Generation | **H2**<br>Electronic and Magnetic Materials | **I2**<br>Biomaterials and Soft Materials and their Application | **O2**<br>Materials for Sustainability | **M2**<br>Nano Materials and Nano Severe Plastic Deformation | 14:00~15:30 |
| Coffee Break 2 | | | | | | | | 15:30~16:00 |
| **D3**<br>Light Metals and Alloys | **K3**<br>High-Entropy Materials and Amorphous Materials | **B3**<br>Advanced Processing of Materials | **G3**<br>Materials for Energy Storage and Generation | **H3**<br>Electronic and Magnetic Materials | **I3**<br>Biomaterials and Soft Materials and their Application | **O3**<br>Materials for Sustainability | **M3**<br>Nano Materials and Nano Severe Plastic Deformation | 16:00~18:00 |
| **POSTER** Session 1 | | | | | | | | 18:00~19:30 |

# **Session** Timetable

## NOVEMBER 21 (Tuesday)

| | 201 A | 201 B | 202 A | 202 B | 203 | Halla A | Halla B |
|---|---|---|---|---|---|---|---|
| 09:00~10:20 | **Plenary** Session 2 : Dr. George T. (Rusty) Gray III (Los Alamos Nat'l Lab. USA)<br>**Plenary** Session 3 : Prof. Matthew Barnett (Deakin University, Australia) | | | | | | |
| 10:20~10:50 | Coffee Break 3 | | | | | | |
| | C4 | J4 | F4 | L4 | N4 | A4 | E4 |
| 10:50~12:30 | Structural Materials for High Temperature | Materials Characterization and in situ/3D/4D Analysis | Thin Films and Surface Engineering | Composite, Coating and Hetero-Materials | Computational Materials and Artificial Intelligence | Advanced Steels and Properties | Additive Manufacturing |
| 12:30~14:00 | **Lunch 2** (Tamna B+C, 5F) | | | | | | |
| 14:00~15:30 | **C5** Structural Materials for High Temperature | **J5** Materials Characterization and in situ/3D/4D Analysis | **F5** Thin Films and Surface Engineering | **L5** Composite, Coating and Hetero-Materials | **N5** Computational Materials and Artificial Intelligence | **A5** Advanced Steels and Properties | **E5** Additive Manufacturing |
| 15:30~16:00 | Coffee Break 4 | | | | | | |
| 16:00~18:00 | **C6** Structural Materials for High Temperature | **J6** Materials Characterization and in situ/3D/4D Analysis | **F6** Thin Films and Surface Engineering | **L6** Composite, Coating and Hetero-Materials | **N6** Computational Materials and Artificial Intelligence | **A6** Advanced Steels and Properties | **E6** Additive Manufacturing |
| 18:00~20:30 | **Banquet** (Tamna Hall B+C, 5F) | | | | | | |

# **Session** Timetable

## NOVEMBER 21 (Tuesday)

| Samda A | Samda B | 301 | 303 A | 303 B | 400 | 401 | 402 | |
|---|---|---|---|---|---|---|---|---|
| **Plenary** Session 2 : Dr. George T. (Rusty) Gray III (Los Alamos Nat'l Lab. USA)<br>**Plenary** Session 3 : Prof. Matthew Barnett (Deakin University, Australia) | | | | | | | | 09:00~10:20 |
| Coffee Break 3 | | | | | | | | 10:20-10:50 |
| **D4**<br>Light Metals and Alloys | **K4**<br>High-Entropy Materials and Amorphous Materials | **B4**<br>Advanced Processing of Materials | **G4**<br>Materials for Energy Storage and Generation | **H4**<br>Electronic and Magnetic Materials | **I4**<br>Biomaterials and Soft Materials and their Application | **O4**<br>Materials for Sustainability | **M4**<br>Nano Materials and Nano Severe Plastic Deformation | 10:50-12:30 |
| **Lunch 2** (Tamna B+C, 5F) | | | | | | | | 12:30~14:00 |
| **D5**<br>Light Metals and Alloys | **K5**<br>High-Entropy Materials and Amorphous Materials | **B5**<br>Advanced Processing of Materials | **G5**<br>Materials for Energy Storage and Generation | **H5**<br>Electronic and Magnetic Materials | **I5**<br>Biomaterials and Soft Materials and their Application | **O5**<br>Materials for Sustainability | **M5**<br>Nano Materials and Nano Severe Plastic Deformation | 14:00~15:30 |
| Coffee Break 4 | | | | | | | | 15:30~16:00 |
| **D6**<br>Light Metals and Alloys | **K6**<br>High-Entropy Materials and Amorphous Materials | **B6**<br>Advanced Processing of Materials | **G6**<br>Materials for Energy Storage and Generation | **H6**<br>Electronic and Magnetic Materials | **I6**<br>Biomaterials and Soft Materials and their Application | **O6**<br>Materials for Sustainability | **M6**<br>Nano Materials and Nano Severe Plastic Deformation | 16:00~18:00 |
| **Banquet** (Tamna Hall B+C, 5F) | | | | | | | | 18:00~20:30 |

# **Session** Timetable

## NOVEMBER 22 (Wednesday)

| | 201 A | 201 B | 202 A | 202 B | 203 | Halla A | Halla B |
|---|---|---|---|---|---|---|---|
| 09:00~10:20 | **Plenary** Session 4 : Prof. Fusheng Pan (Chongqing University, China)<br>**Plenary** Session 5 : Prof. Tadashi Furuhara (Tohoku University, Japan) | | | | | | |
| 10:20~10:50 | Coffee Break 5 | | | | | | |
| 10:50~12:30 | **C7**<br>Structural Materials for High Temperature | **J7**<br>Materials Characterization and in situ/3D/4D Analysis | **F7**<br>Thin Films and Surface Engineering | **L7**<br>Composite, Coating and Hetero-Materials | **N7**<br>Computational Materials and Artificial Intelligence | **A7**<br>Advanced Steels and Properties | **E7**<br>Additive Manufacturing |
| 12:30~14:00 | **Lunch 3** (Tamna B+C, 5F) | | | | | | |
| 14:00~15:30 | **C8**<br>Structural Materials for High Temperature | **E8-2**<br>Additive Manufacturing | **F8**<br>Thin Films and Surface Engineering | **L8**<br>Composite, Coating and Hetero-Materials | **N8-1**<br>Computational Materials and Artificial Intelligence | **A8**<br>Advanced Steels and Properties | **E8-1**<br>Additive Manufacturing |
| 15:30~16:00 | Coffee Break 6 | | | | | | |
| 16:00~18:00 | **C9**<br>Structural Materials for High Temperature | **E9-2**<br>Additive Manufacturing | **F9**<br>Thin Films and Surface Engineering | **L9**<br>Composite, Coating and Hetero-Materials | **N9-1**<br>Computational Materials and Artificial Intelligence | **A9-1**<br>Advanced Steels and Properties | **E9-1**<br>Additive Manufacturing |
| 18:00~19:30 | **POSTER** Session 2 | | | | | | |

# **Session** Timetable

## NOVEMBER 22 (Wednesday)

| Samda A | Samda B | 301 | 303 A | 303 B | 400 | 401 | 402 | |
|---|---|---|---|---|---|---|---|---|
| **Plenary** Session 4 : Prof. Fusheng Pan (Chongqing University, China)<br>**Plenary** Session 5 : Prof. Tadashi Furuhara (Tohoku University, Japan) | | | | | | | | 09:00~10:20 |
| Coffee Break 5 | | | | | | | | 10:20-10:50 |
| **D7**<br>Light Metals and Alloys | **K7**<br>High-Entropy Materials and Amorphous Materials | **B7**<br>Advanced Processing of Materials | **G7**<br>Materials for Energy Storage and Generation | **H7**<br>Electronic and Magnetic Materials | | **O7**<br>Materials for Sustainability | **M7**<br>Nano Materials and Nano Severe Plastic Deformation | 10:50-12:30 |
| **Lunch 3** (Tamna B+C, 5F) | | | | | | | | 12:30~14:00 |
| **D8**<br>Light Metals and Alloys | **K8**<br>High-Entropy Materials and Amorphous Materials | **B8**<br>Advanced Processing of Materials | **G8**<br>Materials for Energy Storage and Generation | **H8**<br>Electronic and Magnetic Materials | **N8-2**<br>Computational Materials and Artificial Intelligence | **O8**<br>Materials for Sustainability | **M8**<br>Nano Materials and Nano Severe Plastic Deformation | 14:00~15:30 |
| Coffee Break 6 | | | | | | | | 15:30~16:00 |
| **D9**<br>Light Metals and Alloys | **K9**<br>High-Entropy Materials and Amorphous Materials | **B9**<br>Advanced Processing of Materials | **G9**<br>Materials for Energy Storage and Generation | **A9-2**<br>Advanced Steels and Properties | **N9-2**<br>Computational Materials and Artificial Intelligence | **O9**<br>Materials for Sustainability | | 16:00~18:00 |
| **POSTER** Session 2 | | | | | | | | 18:00~19:30 |

# **Session** Timetable

## NOVEMBER 23 (Thursday)

| | Halla A | Halla B | Samda A | Samda B | 301 | 303 A | 303 B | 401 |
|---|---|---|---|---|---|---|---|---|
| | A10-1 | E10-1 | D10 | K10 | B10 | E10-2 | A10-2 | P1 |
| 9:00~10:20 | Advanced Steels and Properties | Additive Manufacturing | Light Metals and Alloys | High-Entropy Materials and Amorphous Materials | Advanced Processing of Materials | Materials for Energy Storage and Generation | Advanced Steels and Properties | 4th KIM-CSM symposium |
| 10:20~10:50 | Coffee Break 7 | | | | | | | |
| 10:50~12:30 | **A11-1** Advanced Steels and Properties | **E11-1** Additive Manufacturing | **D11-1** Light Metals and Alloys | **K11** High-Entropy Materials and Amorphous Materials | **D11-2** Advanced Processing of Materials | **E11-2** Materials for Energy Storage and Generation | **A11-2** Advanced Steels and Properties | **P2** 4th KIM-CSM symposium |
| 12:30~14:00 | **Lunch 4** (Tamna B+C, 5F) | | | | | | | |
| 14:00~15:30 | **A12** Advanced Steels and Properties | | **D12-1** Light Metals and Alloys | **K12** High-Entropy Materials and Amorphous Materials | **D12-2** Advanced Processing of Materials | | | **P3** 4th KIM-CSM symposium |
| 15:30~16:00 | **Closing** Ceremony (Halla Hall B, 3F) | | | | | | | |

# **Plenary** Session

## Session 1

**Speaker :** Prof. Byeong-Joo Lee (POSTECH)

**Chair :** Dr. Zenji Horita (Kyushu Institute of Technology)

**Time & Place :** November 20 (Mon), 9:40-10:20, Tamna Hall A, 5F

## Session 2

**Speaker :** Dr. George T. (Rusty) Gray III (Los Alamos Nat'l Lab.)

**Chair :** Prof. Yuntian Zhu(City University Of Hong Kong)

**Time & Place :** November 21 (Tue), 9:00-9:40, Tamna Hall A, 5F

## Session 3

**Speaker :** Prof. Matthew Barnett (Deakin University)

**Chair :** Prof. Jeong Whan Yoon(KAIST)

**Time & Place :** November 21(Tue), 9:40-10:20, Tamna Hall A, 5F

## Session 4

**Speaker :** Prof. Fusheng Pan (Chongqing University)

**Chair :** Prof. Kwang Seon SHIN (Seoul National University)

**Time & Place :** November 22(Wed), 9:00-9:40, Tamna Hall A, 5F

## Session 5

**Speaker :** Prof. Tadashi Furuhara (Tohoku University)

**Chair :** Prof. Irene Beyerlein (University of California Santa Barbara)

**Time & Place :** November 22 (Wed), 9:40-10:20, Tamna Hall A, 5F

# Plenary Session 1




## Byeong-Joo Lee

Professor, Pohang University of Science and Technology (POSTECH)

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••• Web: http://cmse.postech.ac.kr


## »EDUCATION

| | | | |
|---|---|---|---|
| Seoul National University | Ph.D | Mater. Sci. & Engineering | 1989 |
| Seoul National University | MS | Mater. Sci. & Engineering | 1986 |
| Seoul National University | BS | Mater. Sci. & Engineering | 1984 |

## »PROFESSIONAL ACTIVITIES

- Professor, Depart. Materials Science & Engineering, POSTECH, (Mar. 2009 to Present)
- Associate Professor, Depart. Materials Science and Engineering, POSTECH, (Mar. 2002 to Feb. 2009)
- Guest Researcher, Div. of Computational Thermodynamics, KTH, Sweden (Jun. 1999 to Aug. 1999)
- Post-Doc., Division of Physical Metallurgy, KTH, Sweden (Jan. 1991 to Dec. 1991)
- Senior Researcher, Principal Researcher, Korea Research Institute of Standards and Science (Sep. 1990 to Mar. 2002)
- Post-Doc., Korea Research Institute of Standards and Science (Sep. 1989 to Aug. 1990)
- Associate Editor of the Journal, CALPHAD (1998 to present)

## »AWARD AND HONORS

- The National Academy of Engineering of Korea, Fellow (2019 ~ )
- The Korean Academy of Science and Technology , Fellow (2017 ~ )
- POSCO Academic Award, KIM (Korean Inst. Metals & Mater.) (2017)
- Best Paper Award, CALPHAD (2011)
- SeAH Academic Award, KIM (2010)
- Selected as a "Recommended Researcher" by the Ministry of Science and Technology, Korea (Nov. 1995 ~ Oct. 1998)
- Young Researcher Award, KIM (1997)
- Best Paper Award, KIM (1994)

## »MAIN SCIENTIFIC PUBLICATION

- "Second Nearest-Neighbor Modified Embedded Atom Method Potential," Phys. Rev. B. (2000).
- "Second Nearest-Neighbor Modified Embedded Atom Method Potentials for BCC Transition Metals," Phys. Rev. B. (2001).
- "Semi-Empirical Atomic Potentials for the FCC metals Cu, Ag, Au, Ni, Pd, Pt, Al and Pb based on First and Second Nearest-Neighbor Modified Embedded Atom Method," Phys. Rev. B. (2003).
- "Prediction of Interface Reaction Products between Cu and Various Solder Alloys by Thermodynamic Calculation," Acta Materialia (1997).
- "Understanding the Physical Metallurgy of the CoCrFeMnNi High-Entropy Alloy: An Atomistic Simulation Study," NPJ Computational Materials (2018).
- "Dislocation binding as an origin for the improvement of room temperature ductility in Mg alloys," Mater. Sci. Eng. A (2018)
- "100 texture evolution in bcc Fe sheets - computational design and experiments," Acta Materialia (2016).
- "A Modified Embedded-Atom Method Interatomic Potential for Ionic Systems: 2NNMEAM+Qeq," E. Lee, K.-R. Lee, M. I. Baskes and B.-J. Lee, Phys. Rev. B. 93, 144110 (2016).
- "Activation of non-basal <c+a> slip in multicomponent Mg alloys," Journal of Magnesium and Alloys (2022).

## »RESEARCH INTERESTS

- Development of Thermodynamic Database:
  TCFE2000, a thermodynamic database for steels, was developed in 1999 in collaboration with the ThermoCalc Group at KTH, Sweden. The database is now updated to cover wider range of materials including high entropy alloys.
- Development of second nearest-neighbor (2NN) MEAM potentials and formalism:
  The 2NN MEAM potential formalism is one of the strongest interatomic potential models especially for multicomponent system, in a sense that individual elements should be described using one common formalism to deal with multicomponent alloy systems and that the 2NN MEAM can be applied to a wide range of elements: fcc, bcc, hcp, diamond and even gaseous elements, without changing its formalism. This formalism was recently further extended into the ionic bonding materials systems.
- Computational Materials and Process Design:
  The computational techniques have been applied to design of various value-added materials and processes including {100} textured electric steels sheets, Mg alloys with room temperature ductility and formability and high entropy alloys with improved strength-ductility balance.

# Computational Materials and Process Design

Byeong-Joo Lee[1], Kyeong-Min Kim[2], Hyeon-Seok Do[2], Jaemin Wang[2], Seok Su Sohn[3], Hyoung Seop Kim[4], Nack Joon Kim[4]

[1] Department of Material Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang 37673, Republic of Korea
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[2] Department of Material Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang 37673, Republic of Korea
Email: lovekm91@postech.ac.kr, hyeonseokdo@postech.ac.kr, wjmpinkiepie@postech.ac.kr

[3] Department of Material Science and Engineering, Korea University, Seoul 02841, Republic of Korea
Email: sssohn@korea.ac.kr

[4] Graduate Institute of Ferrous Technology, Pohang University of Science and Technology (POSTECH), Pohang 37673, Republic of Korea
Email: hskim@postech.ac.kr, njkim@postech.ac.kr

Computational approaches such as first-principles calculations, atomistic simulations, phase field simulations, computational thermodynamics and finite element method simulations are widely used in the metals and materials community. In this talk, a successful example of computational materials and process design - design of highly value-added {100} textured steel sheets - will be outlined, focusing on ways to utilize the results of computational approaches. It will be emphasized that it is more important to clarify the governing mechanism of materials phenomena from the effects of individual experimental variables on simulation results rather than make an effort to obtain good agreement between simulations and experiments with phenomenological issues. Efforts to design novel HEAs using two different approaches will also be presented, one based on multi-strengthening mechanisms and the other using a neural network modelling. In the first approach, the strength of Co-Cr-Fe-Mn-Ni based HEA is improved via various strengthening mechanisms, such as solid solution strengthening, TRIP, and precipitation hardening. We use CALPHAD-type thermodynamic calculations (calculation of phase equilibria, free energy difference between FCC and metastable solid solution phases) and precipitation kinetics. In the second approach, first we suggest a novel and robust neural network model to relieve the burden of searching vast compositional space. Then, we inverse-predict the process condition to obtain HEAs with good mechanical properties. Finally, we conduct experimental verification on the designed HEAs to prove the validity of the model and alloy design method. The strengths and limitations of each approach will be discussed.

**Keywords:** Atomistic Simulation, Thermodynamic Calculation, Machine-Learning, Alloy Design, Process Design.



# George T. (Rusty) Gray III

Lab Fellow – Los Alamos National Laboratory (LANL)

••• E-mail: rusty@lanl.gov

## »EDUCATION

| | | | |
|---|---|---|---|
| Carnegie-Mellon University | PhD | Metallurgical Engineering | 1981 |
| South Dakota School of Mines | MS | Metallurgical Engineering | 1977 |
| South Dakota School of Mines | BS | Metallurgical Engineering | 1976 |

## »PROFESSIONAL ACTIVITIES

- September 2012-present : Scientist 6; LANL
- September 2002-present : Laboratory Fellow, LANL
- Jan. 1985-Sept. 2003 : Team Leader and Technical Staff Member, LANL
- Jan. 1982-Nov. 1984 : Post-doctoral Fellowship
  TECHNISCHE UNIVERSITAET HAMBURG-HARBURG, Germany

## »AWARD AND HONORS

- 1997 - Elected Fellow of ASM International
- 1998 - Elected Life Member Clare Hall, Cambridge University, U.K.
- 2002 - Named Fellow of Los Alamos National Laboratory
- 2006 - Elected Fellow of the American Physical Society (APS)
- 2010 - President of The Minerals, Metals, and Materials Society (TMS)
- 2013 - Inducted as Fellow of TMS (The Minerals, Metals, and Materials Society)
- 2017 - Inducted into National Academy of Engineering (NAE)
- 2018 - Awarded the DYMAT John Rinehart Award by the European DYMAT Association
- 2019 - Awarded the APS -- 2019 George E. Duvall Shock Compression Science Award
- 2020 - Awarded-American Ceramic Society ICACC Lecture
- 2021 - Awarded the 2021 SDSM&T Distinguished Alumni Award
- 2023 - Awarded the ASM Edward DeMille Campbell Lecture Award

## »MAIN SCIENTIFIC PUBLICATION

- Over 490 publications; H-Index of 70; > 17,000 citations

## »RESEARCH INTERESTS

- Processing / Structure / Property / Performance relationships during the deformation of materials, in particular in response to high-strain-rate and shock deformation.

# Dynamic Behavior of Additively Manufactured Materials

George T. (Rusty) Gray III[1]

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Materials Physics and Applications Division
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## Abstract

Additive manufacturing (AM) has provided a new paradigm of control not only of material microstructure but also of structural assembly. The promise of AM lies in tailoring properties through this exquisite microstructural and topological design and fabrication, and the possibility of "metamaterial" properties simply not possible through most conventional manufacturing. Relevant to mechanical properties and dynamic performance, the application of AM has resulted in many examples in which control of deformation mechanics and structural instabilities has led to novel properties, such as high strength-to-weight ratios, tailored thermal management, and auxetic properties. This talk will provide an overview of the dynamic behaviors of additively manufactured metals, and provide a perspective on the current challenges in AM for dynamic loading environments and future directions in the area.

**TMS Plenary Speaker**

Keywords: Additive Manufacturing, Dynamic Material Behavior, Structure/Property Behavior, High-Strain Rate, Shock-Loading.

# Plenary Session 3




## Matthew Barnett

ARC Laureate Professor, Deakin University

••• E-mail: barnettm@deakin.edu.au
••• Web: www.deakin.edu.au/ifm


## »EDUCATION

| | | | |
|---|---|---|---|
| McGill University, Montreal | Ph.D | Metallurgical Engineering | 1997 |
| RMIT University | BEng | Metallurgical Engineering | 1994 |

## »PROFESSIONAL ACTIVITIES

- ARC Laureate Professor, Deakin University, September 2022-present
- Director, mineAlloy ARC Training Centre, Deakin University, 2016-present
- Director, Institute for Frontier Materials, Deakin University, 2017-2022

## »AWARD AND HONORS

- ARC Laureate Professor, 2022
- TMS Brimacombe Medalist, 2016
- Alfred Deakin Professorship, 2014
- ARC Future Fellowship, 2011
- ARC QEII Fellowship, 2004

## »MAIN SCIENTIFIC PUBLICATION

- Over 18,000 citations from over 260 publications
- Key recent publication:

Barnett, M.R et al. "A scrap-tolerant alloying concept based on high entropy alloys" (2020) Acta Materialia, 200, pp. 735-744.

## »RESEARCH INTERESTS

- Physical metallurgy, alloy development
- Integrating societal implications into alloy design
- Redesigning alloys for a more circular economy

# Some Material Challenges for a Sustainable Circular Economy

Matthew Barnett

[1] *Institute for Frontier Materials, Deakin University, Geelong, Victoria 3321, Australia*
*Email: barnettm@deakin.edu.au*

## Abstract

Materials that loop. It's an attractive concept. But there are many reasons why materials won't allow themselves to be nicely looped around the economy. And in critical cases, our forecast material demand far exceeds the likely availability of existing stocks, so virgin material will remain in high demand. Still, seeking to foster a more circular economy - one that is sustainable - is a noble goal. One simple reason is that a circular economy promises to preserve the value of the energy we have already spent in creating the materials we use. The present talk will examine a number of challenges and some potential solutions and pathways for enhancing material circularity with a firm view on total energy demands and the concomitant carbon emissions. The focus will be largely on metal alloys but the steep challenge faced by carbon fibre composites will also be considered. The simple case will be (re)made that extending material lifetime must play a critical role in any attempt to move towards a more circular economy. Low emission, low embodied energy, highly distributed technologies are also desirable. And so it is possible that additive manufacturing may be able to play a role. An example of this will be presented.

**Keywords:** circular economy, low emission technologies, recycling, alloy development

# Plenary Session 4



## Fusheng Pan


- Academician, Chinese Academy of Engineering, China
- Chairman, Chongqing Association for Science & Technology, China
- President, International Mg Society
- Vice President, Chinese Materials Research Society (C-MRS), China
- Director, Chongqing Center of Chinese Academy of Engineering, China
- Director and Professor, National Engineering Research Center for Magnesium Alloys (Chongqing University), China

••• E-mail: fspan@cqu.edu.cn
••• Web: http://ccmg.cqu.edu.cn


## »EDUCATION

**1991-1994:** PhD in Materials Science & Engineering, Northwestern Polytechnical University, China;
**1982-1985:** MSc in Materials, Chongqing University, China;
**1978-1982:** BSc in Powder Metallurgy, Hefei University of Technology, China

## »PROFESSIONAL ACTIVITIES

### In China:

- 2018-now: Director, Chongqing Center of Chinese Academy of Engineering, China
- 2017-now: Academician, Chinese Academy of Engineering, China
- 2007-now: Professor and Director, National Engineering Research Center for Magnesium Alloys (Chongqing University), Chongqing, China;
- 2008-2018: President, Chongqing Academy of Science & Technology, Chongqing, China;
- 1998-2012: Director-General, Chongqing Science & Technology Commission, Chongqing Government, Chongqing, China;
- 1994-1998: Professor and Vice Dean, Graduate School, Chongqing University, Chongqing, China;
- 1993-1994: Professor and Vice Chair, Department of Metallurgy and Materials, Chongqing University, Chongqing, China;
- 1989-1992: Associate Professor, Department of Metallurgy and Materials, Chongqing University, Chongqing, China;
- 1985-1989: Teacher, Department of Metallurgy and Materials, Chongqing University, Chongqing, China

### In foreign countries:

- 2015-now: Honorary Professor, University of Queensland, Australia
- 2006-2007: Visiting Professor, College of Materials, Queen Mary College, UK
- 2002-2003: Guest Scientist, Faculty of Engineering, Chiba University, Japan

- 1995-1996: Guest Scientist, National Materials Testing Institute, Stuttgart University, Germany;
- 1991-1993: Visiting Professor, Department of Materials, Oxford University, UK.

## »AWARD AND HONORS

- 2017: 1st Prize for Scientific and Technological Invention of Chinese Materials Research Society
- 2016: Awards of Excellence International Magnesium Association
- 2013: 1st S&T Prize by the Ministry of Education of China
- 2011: the National S&T Prize by the State Council of China
- 2010: 1st S&T Prize by the Ministry of Education of China
- 2009: the Outstanding Scientist Prize of China by the Ministry of S&T of China
- 2008: HLHL S&T Innovation Prize by HL HI Foundation (The most famous non-government S&T Prize in China)
- 2007: 1st S&T Prize by the Ministry of Education of China
- 2004: the National S&T Prize by the State Council of China
- 2003: 1st S&T Prize by the Ministry of Education of China
- 2001: Dupont S&T Innovation Prize (USA)
- 1998: the National S&T Prize by the State Council of China.

## »MAIN SCIENTIFIC PUBLICATION

- Over 800 journal publications in Acta Materialia, Corrosion Science, Metallurgical and Materials Transaction, Materials Science & Engineering, Script Materialia, Journal of Materials Science, Journal of Alloys & Compounds, Journal of Materials Research, Materials & Design and other journals.
- Over 180 invention patents and 12 other patents.
- 12 books (two in English, the others in Chinese)
- Over 20 ISO, GB/T and industrial standards
- The detailed lists for selected publications can be found in the attached documents. In the past decade, the number of published papers in SCI journals on magnesium alloys ranks 1st in the world, and the number of patents on magnesium alloys ranks 1st in China.

## »RESEARCH INTERESTS

- Magnesium alloy, aluminum alloy, energy storage materials, biomaterials, composite materials, powder metallurgy, near net shape casting, recycling of light alloys and tool steels and so on.

# Opportunities and challenges for the development of magnesium industry under the dual carbon background

Fusheng Pan

*National Engineering Research Center for Magnesium Alloys, Chongqing University, Chongqing 400045, China*
*Email: fspan@cqu.edu.cn*

Energy conservation, emission reduction, and energy transformation are important ways to achieve the dual carbon goals. Magnesium based materials are energy-saving and energy storage materials with excellent performance, and have great potential for application in energy conservation, emission reduction, and energy transformation. This report introduces the current development status and latest progress of magnesium alloy lightweight materials and magnesium based energy storage materials. The opportunities and challenges faced in the large-scale application of magnesium alloy lightweight materials and magnesium based energy storage materials are discussed. As the most promising lightweight metal material, magnesium alloys exhibit very high specific strength. Among them, the strength of the new cast magnesium alloy has reached over 400MPa, and the strength of the new ultra-high strength deformed magnesium alloy has reached over 550MPa. As a new generation of energy storage materials, magnesium based materials show excellent performance for energy storage with low cost, high safety, and low environmental cost. Among them, the solid hydrogen storage density of magnesium based materials has exceeded 7%wt, and the comprehensive performance of magnesium batteries has approached the level of lithium iron phosphate battery. The report also introduces typical application fields of magnesium alloy lightweight materials, magnesium hydrogen storage materials, and magnesium batteries. The magnesium industry is expected to become one of the most promising industries in the future.

**Keywords:** magnesium alloys, magnesium batteries, hydrogen storage, lightweight, energy storge

# Plenary Session 5




## Tadashi Furuhara

Professor, Institute for Materials Research, Tohoku University

**E-mail:** tadashi.furuhara.c3@tohoku.ac.jp


## »EDUCATION

| | | | |
|---|---|---|---|
| Carnegie Mellon University, USA | Ph.D | Metallurgical Engineering & Materials Science | 1989 |
| Kyoto University, Japan | ME | Metal Science & Technology | 1985 |
| Kyoto University, Japan | BE | Metal Science & Technology | 1983 |

## »PROFESSIONAL ACTIVITIES

- Research Associate, Department of Metal Science and Technology, Kyoto University, Japan (October 1989 to July 1997)
- Associate Professor, Department of Materials Science and Engineering, Kyoto University, Japan (August 1997 to September 2005)
- Professor (October 2005 to Present.), Director (April 2020 to March 2023), Institute for Materials Research, Tohoku University, Japan
- Vice president: The Japan Institute of Metals and Materials (April 2013 to April 2016)
- President: The Iron and Steel Institute of Japan (April 2022 to Present.)
- Member: Phase Transformations Committee, Materials Processing & Manufacturing Division, TMS (February 2002 to Present.), Steel Committee, Structural Materials Division, TMS (December 2016 to Present.)
- Editor: Acta Materialia and Scripta Materialia, Elsevier (January 2017 to Present.)

## »AWARD AND HONORS

- The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Prizes for Science and Technology, Research Category (2023)
- PTM2022 Hillert - Cahn Award (2022)
- Scientific Achievement Merit Prize, The Iron and Steel Institute of Japan (2020)
- THERMEC'2018 Distinguished Award (2018)
- Meritorious Honor Award (Hayashi Award), The Japan Society for Heat Treatment (2017)
- Tanigawa-Harris Award, The Japan Institute of Metals and Materials (2015)
- Technology Award, The Japan Society of Spring Engineers (2009)

- Technology Award, The Japan Titanium Society (2006)
- Vanadium Award, Institute of Materials, Minerals and Mining, UK (2005, 2016, 2022)
- Sawamura Award, The Iron and Steel Institute of Japan (2003, 2008, 2014, 2017)
- Tawara Award, The Iron and Steel Institute of Japan (2003, 2008, 2014, 2017)
- Best Paper Award, The Japan Institute of Metals (1996, 2000, 2009)
- Best Paper Award, The Japan Society for Heat Treatment (2020)

## »MAIN SCIENTIFIC PUBLICATION


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## »RESEARCH INTERESTS

- Thermodynamics, kinetics and crystallography of phase transformations in metallic materials
- Microstructure control by thermomechanical processing in ferrous and non-ferrous alloys
- Surface hardening treatment of steels

# Exploring for the Future of Steel Science

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## Abstract

Steel continues to be one of the most important materials with mass production and sustainability to maintain our future society. However, recent changes in natural and international environments requires us big challenges both scientifically and industrially in many aspects. Thus, it is necessary to solve such difficult tasks with multidisciplinary and new state of arts of materials science and technology.

Recent developments in multiscale microstructure characterization and computational materials science have enabled us to advances and accelerate the materials research at different levels from those in the last century. In this lecture, recent trends in the major research concepts in structural materials in Japan are first summarized focusing in particular on steel. Then, examples of advanced high strength steels research establishing much deeper understanding in microstructure development and resultant properties are introduced, and finally future perspectives of steel science and technology will be briefly discussed.

**Keywords:** Microstructure and Properties, Advanced Characterization, Computational Materials Science, Data-driven Research, Elemental Strategy

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 1

November 20

10:50-12:30

# Technical **Oral Session _ Session 1**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 1 (A1)** **10:50 - 12:30, Nov. 20**

**Chair :** Byoungchul Hwang (Seoul National University of Science and Technology) Halla Hall A, 3F

10:50-11:20 **K-A0337** **[Keynote] Mechanisms of dislocation multiplication and nano-twin formation in a thermally cycled Fe-17Mn alloy**
Young-Kook Lee (Yonsei University, Korea)

11:20-11:40 **I-A0858** **[Invited] Negative strain-rate sensitivity in advanced high-strength steel: Critical role of carbon**
Mingxin Huang (University of Hongkong, China)

11:40-12:00 **I-A0114** **[Invited] Strengthening contributions of dislocations and twins in warm-rolled TWIP steels**
Yizhuang Li (Northeastern University, China)

12:00-12:15 **O-A1012** **DSA-induced twinning in a ferritic low-density steel**
Mahdi Aghaahmadi (Hanbat National University, Korea)

12:15-12:30 **O-A0264** **Characterization of serration behavior in transformation-induced plasticity (TRIP) steels by digital**
Myeong-heom Park (Kyoto University, Japan)

# Mechanisms of dislocation multiplication and nano-twin formation in a thermally cycled Fe-17Mn alloy

**Young-Kook Lee[1]**, Jin-Young Lee[2], Jin-Sung Hong[3]

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## Abstract

Mechanisms of dislocation multiplication and nano-twin formation occurring during γ ↔ ε thermal cycling were investigated using Fe-17Mn alloy. Dislocations were introduced in γ austenite at grain boundaries and inside the grains during thermally-induced $\gamma \leftrightarrow \varepsilon$ transformations. Dislocations near grain boundaries were the dislocations, which constituted ε martensite and returned to grain boundaries during $\varepsilon \rightarrow \gamma$ reverse transformation, and forest dislocations introduced by plastic deformation during $\gamma \leftrightarrow \varepsilon$ transformations. Dislocations inside the grains formed by the impingement between two ε platelets and by the branching of a new ε platelet from a pre-existing ε platelet. In addition, nano-twins were observed in the γ grains after $\varepsilon \rightarrow \gamma$ reverse transformation. The nano-twinned γ structure resulted from stacking faults inside ε platelets because the stacking faults have a twin relationship with the prior γ. Therefore, the yield strength at the peak temperature of thermal cycling increased with the number of thermal cycling due to the increases in not only dislocation density but also nano-twins.

*Keywords: Martensitic transformation, Stacking faults, Dislocation, Transmission electron microscopy, Nano-twins*

# Negative strain-rate sensitivity in advanced high-strength steel: Critical role of carbon

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## Abstract

Advanced high-strength steel (AHSS) with positive strain-rate sensitivity (SRS) are highly desired for industry. However, negative SRS is occasionally observed, particularly in state-of-the-art 3rd-generation AHSS. Using a room temperature quenching and partitioning (RT-Q&P) steel as model material, the present work aims to reveal the origin of negative SRS in AHSS. The strain rate dependent mechanical properties of the RT-Q&P steel were characterized by a series of continuous tensile tests over wide range of strain rates from $10^{-5}$ $s^{-1}$ to 600 $s^{-1}$. The flow stress after yielding exhibits abnormal negative SRS. The interrupted tensile tests at $10^{-3}$ $s^{-1}$ and 600 $s^{-1}$ were performed, along with synchrotron X-ray diffraction measurements, to reveal the strain rate dependent microstructure evolutions, including the evolutions of martensitic transformation and dislocation densities. It was found that similar martensitic transformation occurs at both $10^{-3}$ $s^{-1}$ and 600 $s^{-1}$, implying that transformation induced plasticity (TRIP) effect is not responsible for the negative SRS. Surprisingly, the dislocation density increases remarkably at $10^{-3}$ $s^{-1}$, while remains constant at 600 $s^{-1}$. On the contrary, the micro-hardness evolutions are nearly identical for both strain rates. The designed interrupted rate-change tests and interrupted high-strain-rate load-unload-load tests were performed to reveal the effect of interstitial carbon on the negative SRS. The Cottrell atmospheres with carbon segregated at dislocations were further confirmed by APT. The origin of negative SRS was finally recognized as the lack of Cottrell atmospheres at high strain rate, which leads to absence of extra carbon dragging force and a lower dislocation density.

*Keywords: Strain-rate sensitivity; Advanced high-strength steel; TRIP; Dislocation density; interstitial carbon.*

# Strengthening contributions of dislocations and twins in warm-rolled TWIP steels

**Yizhuang Li**[1], Zhiyuan Liang[2], Mingxin Huang[3]

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## Abstract

A twinning-induced plasticity (TWIP) steel was processed by warm rolling with different reduction ratios to elevate yield strength while maintaining considerable ductility. To investigate the effect of prior warm rolling on the deformation mechanisms during subsequent tensile straining, the contributions of individual strengthening mechanisms to the tensile flow stress of the as-received (AR) and warm-rolled (WR) steels were decoupled, based on the measured dislocation density evolutions determined by synchrotron X-ray diffraction (XRD) experiments. Whereas dislocation multiplication invariably governs the maximum flow stress of the AR and WR steels, deformation twinning becomes increasingly important for the strain hardening of steels with larger worm rolling reductions. In addition, twinning kinetics is enhanced by the pre-existing high dislocation densities caused by warm rolling, leading to an enhancement of twinning-induced hardening. The present work provides further insight into the influence of warm rolling on the deformation mechanisms of TWIP steels.

*Keywords: TWIP steel; Warm rolling; Dislocation density; Deformation twinning; Synchrotron X-ray diffraction*

# DSA-induced twinning in a ferritic low-density steel

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## Abstract

It is widely accepted in the literature that, in the case of ferritic steels, the occurrence of dynamic strain aging (DSA) would deteriorate the tensile properties of those alloys. However, in the present study, it is reported that DSA is capable of triggering the deformation twinning in a high SFE Fe-Mn-Al-C ferrite-base low-density steel, and as a result, a higher amount of DSA at a specific temperature range could result in a higher amount of the uniform elongation of the subjected steel. The obtained stress-strain curves, from room temperature (RT) up to 400 °C, exhibit significant serrated flow behavior, while the serrations disappear at 500 °C. It is shown that these serrations signify the occurrence of DSA in this alloy based on three well-known signs: the serrated flow behavior, the plateau in strain-hardening rate, and the negative strain rate sensitivity in the specified temperature range (RT to 500 °C). The frequency of fluctuations in the stress-strain curves, which is accepted evidence of the intensity of DSA occurrence, was increased from RT to 200 °C. Surprisingly, however, not only the total elongation was not decreased, but also it was increased from 20% at RT to 36% at 200 °C, which is an unexpected behavior due to the higher amount of DSA phenomena at 200 °C, resulting in the formation of stable stacking faults in such a high SFE alloy. A detailed discussion on the strain-hardening mechanisms is presented in using electron backscattered diffraction (EBSD) and transmission electron microscopy (TEM) analysis.

*Keywords: Low-density steel; Dynamic strain aging; Twinning; TWIP; Transmission electron microscopy*

# Characterization of serration behavior in transformation-induced plasticity (TRIP) steels by digital image correlation (DIC) technique

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**Abstract**

Transformation-induced plasticity (TRIP) steels exhibit superior combinations of strength and ductility due to their excellent strain-hardening ability associated with deformation-induced martensitic transformation (DIMT). Besides such a good strength-ductility balance, TRIP steels show unique tensile behavior that exhibits serrated flow on their stress-strain curves. In general, serration behavior has been understood in terms of the dynamic strain aging (DSA) effect resulting from strong interaction between mobile dislocations and solid solution atoms, and it may accompany strain-localized bands, so-called Portevin-Le Chatelier (PLC) bands in the tensile specimen. For revealing underlying reason for the occurrence of serration in carbon-containing TRIP steels, the DIMT effect should also be taken into account as well as DSA effect, because DIMT accompanying shear strain with a volume expansion may contribute to a significant change in the global flow stress. In the present study, we aim to clarify the relationship between serration and PLC banding associated with martensitic transformation kinetics in a Fe-24Ni-0.3C TRIP steel with a fully recrystallized austenite single-phase structure having an average grain size of 35 μm. A significant increase in the martensite volume fraction was observed at a tensile strain of 0.2, around which the serration was changed into more frequently oscillated shape. The digital image correlation (DIC) method for local strain analysis revealed that the propagation of PLC bands dramatically changed by martensitic transformation. The degree of strain localization within the PLC band became strong, and its propagation manner became discontinuous from the tensile strain of 0.2 at which martensitic transformation was accelerated.

*Keywords: Serration behavior; Transformation-induced plasticity; Digital image correlation; mechanical properties; heterogeneous deformation.*

# Technical **Oral Session _ Session 1**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 1 (B1)** **10:50 - 12:25, Nov. 20**

**Chair :** Eun Soo Park (Seoul National University), Yukinobu Natsume (Akita University) 301, 3F

10:50-11:20 **K-B0539** **[Keynote] Predictive multiscale modelling and simulation based on processing-microstructure-properties relationship**
Myoung-Gyu Lee (Seoul National University, Korea)

11:20-11:40 **I-B0384** **[Invited] Application of data assimilation for heat-transfer parameter estimation and high-precision casting simulation**
Yukinobu Natsume (Akita University, Japan)

11:40-11:55 **O-B0498** **Extended Discrete Element Method (XDEM) as a Unified Simulation Platform for Highly Resolved Analysis of Steelmaking Furnaces**
Bernhard Peters (University of Luxembourg, Luxembourg)

11:55-12:10 **O-B0363** **Enhancing formability of FeSi6.5 steel by anodic polarization**
Feng Ye (University of Science and Technology Beijing, China)

12:10-12:25 **O-B0598** **Low-temperature toughness of advanced high-strength steels under plane-strain deformation**
Zeran Hou (Tongji University, China)

# Predictive multiscale modelling and simulation based on processing-microstructure-properties relationship

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## Abstract

The mechanical properties of materials highly depend on their microstructure characteristics which originate from manufacturing processing. Also, the performance of the products or parts made of the materials are related to the complex loadings and environments where they are exposed to. The example of the first issue is the formability or fracture of metals under multiaxial deformation paths and the later includes the recent challenge with the effect of hydrogen on the (delayed) fracture in high strength steels. There have been numerous experimental efforts to understand the link between mechanical properties and microstructures, which provide insight into the material design concepts for improving the performance. Meanwhile, as an alternative to the experiment-based approach which is often time- and cost-consuming, numerical methods have drawn significant attention for predicting mechanical properties of materials at various length scale: multi-scale modelling and simulation approach. In this study, a computational strategy for integrating the processing-microstructure-mechanical properties & performance is highlighted for structural metals. The model developments aim to be highly predictive, not just focused on qualitative analysis, so that they can be utilized for replacing the conventional experimental material characterization at both macro- and meso-scale with high fidelity. As examples, the developed integrated multiscale model is applied to the prediction of anisotropy and formability of metal sheets, the fatigue lifetime under rolling contact, and understanding the microstructure effect on hydrogen transport and the resultant hydrogen embrittled damage in steels.

*Keywords: Multiscale modelling, mechanical properties, microstructure, damage, hydrogen embrittlement*

# Application of data assimilation for heat-transfer parameter estimation and high-precision casting simulation

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## Abstract

Solidification analysis is important for accurately predicting the casting process. Appropriate physical properties of materials and heat-transfer parameters are required for high-precision casting simulations. In particular, parameters such as heat-transfer coefficient (HTC) and thermal conductivity (TC) strongly affect the results of casting simulation. However, because HTC is not a parameter determined uniquely by the material, it is usually estimated by the trial-and-error method, which has the disadvantage of being time consuming. Because TC is affected by convection during solidification, accurate simulations cannot be performed in some cases even if the reported values are used. To overcome these problem, we have developed a method for easily estimating the HTC and TC in casting by combining data assimilation and casting simulation. In particular, the proposed method can reproduce one-dimensional temperature distribution in unidirectional casting with high accuracy. This method can easily and accurately estimate the time-dependent HTC and TC. In addition, we propose a method to simultaneously estimate multiple HTCs and TC to reproduce three-dimensional temperature distribution in casting with high accuracy. We performed casting experiments for Al-Si and Sn-Bi alloys and measured the temperature at multiple points in the cast and mold to obtain a cooling curve. Two cooling curves located near the casting wall were used to estimate HTCs using data assimilation. Results confirmed that all cooling curves could be reproduced with high accuracy and high-precision casting simulation was possible.

*Keywords: Data assimilation; Heat transfer coefficient; Thermal conductivity; Solidification; Casting simulation.*

# Extended Discrete Element Method (XDEM) as a Unified Simulation Platform for Highly Resolved Analysis of Steelmaking Furnaces

**Bernhard Peters**[1]

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**Abstract**

Currently, steelmaking undergoes transition form traditional technologies of a blast furnace to greener alternatives such as Midrex and Energiron. Although a blast furnace is still the most applied reactor technology for stellmaking, a strong urge for alternative technology exists mainly to comply with stricter environmental limitations and to make steelmaking sustainable. Prototyping of these reactors is impossible due to their shear size so that simulation technologies are more than welcomed to support design and analyse operation. The XDEM Advanced simulation platform addresses these requirements by an innovative and novel technique that relies on a coupled Euler-Lagrange framework. While the granular material in a blast, Midrex or Energiron furnace is treated as discrete entities that undergo motion and are characterised by its thermodynamic state, the interstitial space between the particulate phase is described by a continuum multi-phase approach for solely a gas phase or a multi-phase environment containing liquid iron or slag in addition. Both discrete and continuous phases exchange mass, energy and momentum. Gaseous species are transferred to support in general the reduction process while heat transfer provides the energy for the chemical reactions. Thus, the technology covers the length scales from particles to the global dimensions of a reactor and yields an unprecedented insight into the underlying physics and chemistry. The predicted results and its analysis is paramount for improved design and operation and supports massively the transitional process of the steel industry.

*Keywords: Extended Discrete Elelement Method (XDEM), CFD, Euler-Lagrange Coupling*

# Enhancing formability of FeSi6.5 steel by anodic polarization

**Feng Ye[1],** Dong Zhao[1], Binbin Liu[1], Yaakov B. Unigovski[2], Emmanuel M. Gutman[2], Roni Shneck[2]

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## Abstract

The effect of anodic polarization on plastic deformation behavior and formability of FeSi6.5 steel at room temperature was experimentally investigated through uniaxial tensile and drawing of wire specimen in sulfuric acid solution with current densities of 0–40 mA/cm$^2$. The formability of the FeSi6.5 steel was significantly improved after the anodic polarization. The plastic elongation of the specimen as an anode in the electrochemical environment was 4.4%–7%, but 2.7% in the air. The softening is mainly attributed to the relief in work hardening caused by surface atomic dissolution. The effects of surface dissolution on dislocation activation in the FeSi6.5 steel are quantitatively studied by analyzing the stress relaxation data using the thermal activation theory of dislocation. The stressed FeSi6.5 steel sample in acid solutions ($H_2SO_4$ or HCl) exhibits a much higher rate of stress reduction with time compared with that in air or deionized water. The analyses reveal the mechanism for the accelerated plastic flow induced by the corrosive medium. The variations of these parameters are related to the relaxation of the stress field of dislocations and the weakening of interaction between slip dislocations and short-range obstacles. The chemomechanical effect, including a reduction in apparent activation energy and a decrease in waiting time for dislocation to obtain sufficient thermal activation energy to cross obstacles, causes an increase in the stress relaxation rate (plastic strain rate). The study confirms that surface dissolution accelerates the plastic flow of metals and supports the view that surface dissolution facilitates dislocation slip.

*Keywords: FeSi6.5 steel, plastic deformation, anodic polarization, Voce equation, stress relaxation rate*

# Low-temperature toughness of advanced high-strength steels under plane-strain deformation

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## Abstract

The exceptional mechanical properties of advanced high-strength steels (AHSS) have rendered them highly desirable in the automotive industry, where they enable vehicle lightweighting and enhance passive safety measures. However, the exploration of AHSSs' low-temperature toughness properties, particularly after cold forming, remains insufficient. This inadequacy arises from the limitations of conventional low-temperature impact tests, which are unsuitable for evaluating the mechanical properties of AHSSs with thin thicknesses below 2mm. Thus, this study aims to investigate the low-temperature toughness of two 1500 MPa grade AHSSs, namely QP1500 and TBF1470, using low-temperature three-point bending based on the VDA 238-100 standard. Interestingly, when subjected to three-point bending at both room temperature (20°C) and low temperature (-40°C), QP1500 exhibited a 4-8% improvement in bending angle after undergoing 0.005 and 0.02 uniaxial tension pre-deformation. In contrast, the bending angle of TBF1470 remained nearly unchanged (0.005) or significantly decreased (0.02) under the same conditions. In other words, the variable strain path enhanced the toughness of QP1500 in the plane strain state. Further investigations revealed that the stability and transformation behaviours of retained austenite in QP1500 during deformation played a crucial role in its bending toughness. As future AHSSs with even higher strengths, such as 2000MPa or even 2400MPa, are developed, the issue of low-temperature toughness may become more pronounced. Consequently, employing low-temperature three-point bending as a reliable and straightforward method for assessing the low-temperature toughness of AHSSs holds considerable promise.

*Keywords: Low-temperature toughness, AHSS, bendability, retained austenite.*

# Technical **Oral Session _ Session 1**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 1 (C1)** **10:50 - 12:25, Nov. 20**

**Chair :** Hyun-Uk Hong (Changwon National University) 201A, 2F

10:50-11:20 **K-C0584** **[Keynote] Mechanically-Driven Localized Phase Transformations at Stacking Faults and New Superalloy Design Strategy**
Yunzhi Wang (The Ohio State University, USA)

11:20-11:40 **I-C1024** **[Invited] High temperature oxidation behavior of 22wt% Cr containing Ferritic stainless steels for SOFC interconnects**
Dong Ik Kim (Korea Institute of Science and Technology, Korea)

11:40-11:55 **O-C0072** **Sensitivity of thickness debit effect on secondary orientation of a 3rd generation single crystal superalloy**
Li Wang (Institute Of Metal Research, Chinese Academy Of Sciences, China)

11:55-12:10 **O-C0378** **New composition standard based on cluster formula for superalloy Inconel 718**
Shuang ZHANG (Dalian Jiaotong University, China)

12:10-12:25 **O-C0423** **Formation of stacking fault MC carbides in Ni-Mo-Cr superalloy**
Li Jiang (Shanghai Institute of Applied Physics (SINAP), Chinese Academy of Sciences, China)

# Mechanically-Driven Localized Phase Transformations at Stacking Faults and New Superalloy Design Strategy

L.S. Feng[1], A. Egan[1], T. Smith[2], S. Baskar[1], M. Ghazisaeidi[1], M.J. Mills[1], **Yunzhi Wang[1]**

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**Abstract**

A new phenomenon has been observed in some Ni-based superalloys where phase transformations occur at and are confined to stacking faults, which we refer to as localized phase transformations (LPTs). Alloys with different types of LPTs are found to have drastically different creep properties. In this presentation, we lay out the thermodynamic principles of LPT and demonstrate that the relative stability of an ordered stacking fault phase (SFP) and its disordered counterpart determines the types of LPT (ordering vs. disordering) at each type of stacking faults and a thermodynamic parameter using the free energies of the bulk counterparts of these SFPs is introduced to evaluate the ordering tendency of SFP at each type of faults. The effect of LPT on shear resistance of subsequent dislocations is investigated using ab initio calculations and the results show that an ordered SFP increases the shearing resistance. Thus, the larger the ordering tendency is, the more significant the LPT hardening is, and the better the creep performance would be. Using this new design criterion, a new LPT-strengthened Ni-base superalloy is developed, which exhibits unprecedented creep performance, even outperform single crystal CMXS-4 in its fine grained polycrystalline form. The work is supported by NSF under the DMREF program.

*Keywords: Stacking Fault, Segregation Transition, Phase Transformation, Superalloys, Creep Deformation.*

# High temperature oxidation behavior of 22wt% Cr containing Ferritic stainless steels for SOFC interconnects

**Dong-Ik Kim**[1], Yoon Seok Ko[1, 2], Byung Kyu Kim[1, 2], Heung Nam Han[2], Kyung-Woo Yi[2]
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## Abstract

To achieve the contradictory objectives of increase in power generation and carbon neutral at the same time, power generation using renewable energy becomes no longer an option but an essential solution. Fuel cells using hydrogen are promising clean power generation tools and Solid Oxide Fuel Cell (SOFC) is regarded as a potential candidate of the power source for buildings and ships because of its high fuel efficiency and fuel diversity. The main reason why the SOFC is not fully commercialized so far is the performance of interconnects material. Interconnects of SOFC play a role of physical separator of hydrogen and oxygen and electrical connector of each unit cells. It should have long term stability at the operating temperature (700-800°C) and high electrical conductivity even in the oxidizing circumstance.

These days the Ferritic stainless steels containing high Cr (~22wt%) and micro alloying of Mn (~0.4wt%) are widely accepted as the SOFC interconnects materials because it forms $Cr_2MnO_4$ spinel oxide which has relatively high conductivity at 700-800°C and stable oxide growth rate and reduced Cr evaporation which is detrimental for cathode performance. To enhance oxidation resistance, rare earth elements such as Lanthanum or Zirconium can be added but exact mechanism to improve oxidation resistance was not fully understood yet.

In this presentation, we would like to elucidate how Lanthanum improve oxidation resistance as well as electrical conductivity in high Cr containing Ferritic stainless steels at high temperature. Even though Lanthanum addition can increase oxide growth rate in the early stage of oxidation, it enhances the inward oxidation and forms convoluted interface between oxide layer and matrix. It improves the adhesion of oxide layer and also electrical conductivity of the oxide layer.

*Keywords: SOFC, interconnects, high temperature oxidation resistance, Lanthanum addition effect*

# Sensitivity of thickness debit effect on secondary orientation of a 3rd generation single crystal superalloy

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## Abstract

To lighten the overall weight of engines and improve cooling efficiency, the air-cooled turbine blades, which have a complicated hollow structure, are composed of sections of various thicknesses. Therefore, the mechanical properties of each blade section will depend on secondary dendrite orientation. The thickness debit effect of creep deformation and rupture properties of a single crystal superalloy plays an important role in the design and durability analysis of advanced areo-engines.

A third generation single crystal superalloy was employed in the present paper. Thin wall samples with different secondary dendrite orientations were machined into different thicknesses and creep tested at 1100 ºC/140 MPa. In order to get the microstructure evolution of samples with different secondary dendrite orientations tube samples with different thicknesses were also prepared via high-throughput concept. Thickness debit effect was found in both groups of samples with secondary dendrite orientation of [100] and [110], while [100] samples show more sensitivity to the change of thickness. For samples of 0.5 mm in thickness, creep rupture life of [100] samples is slight shorter than [110] samples. For 1.5 mm samples opposite results were obtained. Microstructure evolution changes of different areas with different secondary dendrite orientations were observed and analyzed in detail.

*Keywords: Superalloy; Creep; Secondary dendrite orientations; Thickness effect; Slip*

# New composition standard based on cluster formula for superalloy Inconel 718

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## Abstract

Superalloys feature multi-elements and complex elemental ranges, which makes the proper composition selection difficult. In fact, more strict composition standards generally apply in practical productions. The objective of this work is to understand and eventually to renew the composition standard via example of the most common grade Inconel 718. We have recently shown that the alloy chemistry originates from a nearest-neighbor cluster [center-shell] plus a few next-neighbor glue atoms, or expressed in cluster formula [center-shell](glue atoms). By grouping the elements into $\overline{Ni}$ = (Ni, Co, Cu, Fe), $\overline{Cr}$ = (Cr, Mn, Si, Mo), and $\overline{Nb}$ = (Nb, Al, Ti), it is found that the reported alloys fall within a narrow composition zone $\overline{Ni}_{11.0\sim13.0}$-$\overline{Cr}_{3.5\sim4.5}$-$\overline{Nb}_1$ confined by cluster formulas of 16 and 18 atoms. This composition zone is also expressed in terms of 288-atom supercluster formulas, $\overline{Ni}_{198\sim208}$-$\overline{Cr}_{63\sim72}$-$\overline{Nb}_{16\sim18}$, which leads to coordinated elemental variations in wt.%: 69.0 ≤ Ni + Co + Cu + Fe ≤ 72.7; 19.8 ≤ Cr + Mn + 1.7Si + 0.6Mo ≤ 22.8; 8.7 ≤ Nb + 3.2Al + 1.9Ti ≤ 9.8. Within this composition zone, $\overline{Ni}_{206}$-$\overline{Cr}_{65.5}$-$\overline{Nb}_{16.5}$ is further pinpointed and validated by our own experiments to possess the optimal match of strength and plasticity both at room temperature and at 923 K. The introduction of such coordinated elemental variations constitutes a new form of composition standard for superalloys, in contrast to conventional ones that usually specify the ranges of individual elements.

*Keywords: Inconel 718 superalloy; Cluster-plus-glue-atom model; Cluster formula; Composition standard; Coordinated elemental variations*

# Formation of stacking fault MC carbides in Ni-Mo-Cr superalloy

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## Abstract

The structural materials used in molten salt reactors (MSRs) require enough high-temperature strength, good chemical compatibility with fuels and irradiation damage resistance. Hastelloy N alloy had been proved to afford the best combination of high temperature strength and corrosion resistance according to its service experiences in the Molten Salt Reactor Experiment (MSRE). However, the serious helium embrittlement of this alloy had been observed in the components from MSRE, which manifested itself as sharp reductions in both the creep-rupture life and the rupture ductility. The addition of MC carbides forming elements (Ti, Nb, Zr and Hf) has been proved to overcome the helium embrittlement problem. Unfortunately, previous studies had not progressed sufficiently to pinpoint the exact role of element addition in bringing about the improved properties. In this study, the nucleation, growth, and degeneration behaviours of MC carbides in the Ni-12Mo-7Cr alloy during the long-term thermal exposure at 650 °C – 850 °C have been investigated. One novel stacking fault MC carbides were observed in the thermal exposed alloy, which are characterized by the dense nano-sized MC carbide particles on the discoid stacking fault from a few microns to dozens of micron range. These MC carbides possess a semi-coherent interface of $(111)_{MC}$ // $(111)_{\gamma}$ with the matrix by the cube-on-cube orientation relationship, which is the microstructure foundation of helium trapping. The formation mechanism, the role of Mo doping and the strengthening effects of stacking fault MC carbides were briefly discussed.

*Keywords: Molten salt, Superalloy, Stacking faults, Carbides, Orientation relationship.*

# Technical **Oral Session _ Session 1**

## **Symposium D :** Light Metals and Alloys

### Light Metals and Alloys 1 (D1) — 10:50 - 12:40, Nov. 20

Chair : Nagaumi Hiromi (Soochow University), Young-Hee Cho (Korea Institute of Materials Science) — Samda Hall A, 3F

10:50-11:20 **K-D1114** **[Keynote] No-tradeoff of Strength and Ductility of Al-Mg Alloys**
Shae Kwang KIM (Korea Institute of Industrial Technology, Korea)

11:20-11:35 **O-D0563** **Enhancement of high-temperature strength in Al-Si alloys by microalloying with transition elements**
Jinxian Huang (Tohoku University, Japan)

11:35-11:55 **I-D0449** **[Invited] Hot deformation behavior of lightweight metals using hot torsion tests**
Soong-Keun Hyun (Inha University, Korea)

11:55-12:10 **O-D0429** **Investigation of the surface pattern formation mechanism of twin-roll cast strip by residual stress measurement**
Yusuke Takayama (National Institute Of Technology (KOSEN), Gunma College, Japan)

12:10-12:25 **O-D0370** **Effects of Cooling Rates on Eutectic Structure and Mechanical Properties of Al-Cu-Si-Mg Quaternary Eutectic Alloy**
Byung-Joo Kim (Korea Institute of Materials Science, Korea)

12:25-12:40 **O-D0272** **Characterization of the effect of Cu-Mg cluster on Al-Cu-Mg alloy hardness**
Shin Fukuda (Hokkaido University, Japan)

# No-tradeoff of Strength and Ductility of Al-Mg Alloys

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**Abstract**

Intrinsic nature of strength and ductility combination (no-tradeoff) of Al-Mg (5xxx series aluminium) alloys, which have up to about 5wt% Mg, will be described. The extended nature of Al-Mg alloys with over 6wt% Mg will be mainly discussed, not only in terms of the maintained strength and ductility combination in the range of 6 to 9wt% Mg but also of improved steel-like formability during cold rolling and for subsequent forming processes such as deep drawing, pressing, and roll forming. The characteristics of high Mg added Al-Mg alloys in the form of flat rolled products can act as breakthrough by down-gauging (lighter than typical Al products) as well as by enhancing carbon neutrality for mobility industries.

*Keywords: aluminium, strength and ductility combination, steel-like formability, down-gauging, carbon neutrality.*

# Enhancement of high-temperature strength in Al-Si alloys by microalloying with transition elements

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## Abstract

Enhancing the high-temperature strength of aluminum alloys is of great significance for expanding their applications. Generally, there is a negative correlation between the diffusion rate and thermal stability of alloying elements. Although vanadium and titanium are one of the transition elements with the lowest diffusion rate in aluminum, the effects of those elements on the high-temperature strength of conventional cast aluminum alloys have not been systematically studied yet. In this study, vanadium and titanium were micro-alloyed into Al-Si cast aluminum alloys, and the effect of vanadium on the high-temperature strength of Al-Si alloys was investigated. The microstructures of the two vanadium-containing alloys were characterized via SEM and TEM, and the relevant mechanisms were discussed. The results show that V-containing intermetallics distribute on the grain boundaries and interconnect with eutectic silicon, thereby significantly improving the high-temperature strength of Al-Si alloys. The simultaneous addition of Ti and V further enhances the high-temperature strength of the alloy, attributed to the increased fraction of V-containing phases. Our work underscores the potential of vanadium element in the development of next-generation heat-resistant aluminum alloys.

*Keywords: high-temperature strength, vanadium, titanium, aluminum alloys*

# Hot deformation behavior of lightweight metals using hot torsion tests

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## Abstract

Due to recent policies prohibiting the sale of internal combustion engines in various countries around the world, competition among advanced automakers to develop eco-friendly cars has been accelerated. In addition, there is an increasing demand for lightweight materials in the transportation industry, driven by the issue of solving traffic congestion in cities through the development of urban air mobility (UAM) based on personal flying vehicles. Consequently, there has been an increase in the need for lightweight metals like aluminum and magnesium, and innovative lightweight alloys that possess exceptional specific strength are being developed. In the case of new alloys, considerable trial and error is required to set appropriate molding temperatures and molding speeds during the molding process, and research on high-temperature deformation behavior is necessary to efficiently carry out the hot working process. When evaluating the deformation behavior of metal materials using high-temperature torsion tests, an efficient testing method with many advantages for simulating actual molding processes, such as the ability to achieve uniform deformation through simple rotation and apply high strain rates to metal materials through pure shear deformation, is utilized. In this study, lightweight metals such as aluminum and magnesium were tested using high-temperature torsion tests, and the high-temperature deformation behavior was evaluated for optimizing hot working processes, including dynamic recrystallization behavior, constitutive equations, and process maps.

*Keywords: aluminum, magnesium, hot deformation, torsion test.*

# Investigation of the surface pattern formation mechanism of twin-roll cast strip by residual stress measurement

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**Abstract**

Twin-roll casting is a unique method that can produce thin strips from molten metal directly. Due to the high cooling rate, fine microstructure improves mechanical properties. And rapid solidification can refine the secondary particles that reduce ductility. So this method is expected to expand the use of recycled Al. However, some unique patterns are formed on the strip surface depending on casting conditions and alloy compositions. One is the periodic pattern which is consisted of periodic shiny and un-shiny regions. The other one is a scaly pattern with un-shiny regions a few millimeters in diameter distributed like fish scales. These patterns are usually harmful to elongation. Previous studies have suggested several methods to reduce these patterns, but the underlying reasons why these patterns form are unknown. Thus, to investigate the pattern formation mechanism, several twin-roll cast strips were conducted for residual stress measurement.

Residual stress was measured by μ-X360s (PULSTEC Corp.). This equipment is based on the cos α method which is the Deby-Scherrer ring analysis method. Measurement strips were pure Al, Al-1 %Mn, Al-7 %Si representing a scary pattern, and Al-5 %Mg representing a periodic pattern. The residual stress distribution and surface patterns corresponded. Especially in Al-5 %Mg, tensile residual stress toward the casting direction was observed in the un-shiny region. In the previous study, the surface crack was observed in the un-shiny region of Al- 5Mg. It means tensile stress generated by solidification shrinkage is the one of reasons to form un-shiny regions and periodic surface patterns.

*Keywords: twin-roll casting, surface pattern, Al alloy, residual stress, cos α method*

# Effects of Cooling Rates on Eutectic Structure and Mechanical Properties of Al-Cu-Si-Mg Quaternary Eutectic Alloy

**Byung-Joo Kim**[1], Hyun-Seok Cheon[1], Jisu-Kim[1], Young-Hee Cho[1], Su-Hyeon Kim[1]*

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**Abstract**

Eutectic or near-eutectic composition alloys, such as Al-Cu-Si-Mg quaternary alloys, offer low melting points and excellent casting properties, providing a balance of high strength and reasonable plasticity. However, previous research on eutectic alloys has primarily focused on binary and ternary alloys (e.g., Al-Cu, Al-Cu-Si, Al-Cu-Mg, Al-Cu-Ag) fabricated through rapid solidification techniques, such as injection casting, suction casting, and directional solidification, to produce ultra-fine microstructures. Quaternary alloys can exhibit lower melting points compared to binary and ternary eutectic alloys, and they can form ultrafine structures through the cooperative growth of multiple eutectic phases. Despite their potential advantages, there is limited information available on the processing conditions and microstructures of quaternary eutectic alloys, such as Al-Cu-Si-Mg.

This study investigates the effects of cooling rates on the eutectic structure and intermetallic lamellar spacing of Al-Cu-Si-Mg quaternary eutectic alloys. Various controlled gravity casting processes with different cooling rates (10 to $10^2$ K/sec) are employed. Cooling rates significantly influence eutectic structures, resulting in morphologies such as dendritic, bimodal, cellular lamellar, and irregular mixtures. Lamellar spacing refines with increasing cooling rates, transitioning from micro-scale to nano-scale, and leads to increased hardness and compression strengths. The research also explores the relationship between eutectic structure and failure mechanical properties, examining changes in eutectic morphology to explain the failure mechanisms of each structural morphology.

*Keywords: Aluminium alloy, Mechanical Properties, eutectic composition alloy, solidification.*

# Characterization of the effect of Cu-Mg cluster on Al-Cu-Mg alloy hardness

**Shin Fukuda**[1], Masato Ohnuma[2],
Junya Kobayashi[3], Goroh Itoh[4], Shigeru Kuramoto[5], Equo Kobayashi[6]

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## Abstract

Strengthening factors in 2000 series aluminum alloys are considered as S-phase, GPB2 zone, and S'' phase. In contrast, it had not been discussed much about the effect of the Cu-Mg co-cluster formed in the early stage of aging on the peak hardness. Therefore, we performed experiments using a high-energy laboratory Small-Angle X-ray Scattering (SAXS) system that allows non-destructive and long-term in-situ observation of the precipitates to investigate the effect of the Cu-Mg co-cluster on the hardness of Al-Cu-Mg alloys.

Al-Cu-Mg alloy specimens with different compositions with a thickness of 1 mm were solution-treated at 480 °C for 1 h, water-quenched and then immediately subjected to SAXS, differential scanning calorimetry (DSC), and micro-Vickers hardness testing. Some specimens were cold-rolled to a thickness of 0.2 mm after quenching, and then immediately subjected to the same characterization methods and testing as above..

The In-situ SAXS observation was performed both on the samples with and without cold rolling during aging at room temperature and 190°C. DSC measurements have been performed from 0 to 400 °C at a heating rate of 5 °C/min both for the unrolled and rolled samples. Micro-Vickers hardness was measured for the unrolled and rolled materials aged at room temperature and 190°C.

Volume fraction, Vf, of Cu-Mg clusters with a diameter of 1 nm has been evaluated from in-situ SAXS measurements. From the change of Vf and hardness, the effect of Cu-Mg clusters on the peak hardness will be discussed in the talk.

*Keywords: aluminum-copper-magnesium alloy, cold rolling, aging, in-situ small-angle X-ray scattering, cluster*

# Technical **Oral Session _ Session 1**

## **Symposium E :** Additive Manufacturing

### Additive Manufacturing 1 (E1) 10:50 - 12:30, Nov. 20

Chair : Bhaskar Majumdar (New Mexico Tech), Kyung Tae Kim (Korea Institute of Materials Science) Halla Hall B, 3F

10:50-11:20 **K-E0199** **[Keynote] Microstructure and High Temperature Mechanical Properties (Tensile, Fatigue, Creep etc.) of Ni-based Superalloys (IN625, 718, 738) manufactured by Laser Powder Bed Fusion Process**
Kee-Ahn Lee (Inha University, Korea)

11:20-11:40 **I-E0177** **[Invited] In-situ synchrotron radiation X-ray diffraction study for understanding strengthening mechanisms of Al–Si alloy manufactured by laser powder bed fusion**
Naoki TAKATA (Nagoya University, Japan)

11:40-12:00 **I-E0664** **[Invited] Balancing mechanical properties and deposition efficiency: the impact of oxidation in laser directed energy deposition**
Shanqing Xu (Swinburne University of Technology, Australia)

12:00-12:15 **O-E0912** **The Effect of Grain Boundary Serration on Improving Hot Ductility of High Entropy Alloy Processed by Selective Laser Melting**
Meng Yun Lee (National Tsing Hua University, Postech, High Entropy Materials Center, Korea)

12:15-12:30 **O-E0939** **Creep and creep mechanism of electron beam-based powder bed fusion 316L stainless steel**
Kwang-Hyeok Lim (Korea Advanced Institute of Science and Technology, Korea)

# Microstructure and High Temperature Mechanical Properties (Tensile, Fatigue, Creep etc.) of Ni-based Superalloys (625, 718, 738) Manufactured by Laser Powder Bed Fusion Process

**Kee-Ahn Lee**[1,*], So-Yeon Park[1], Kyu-Sik Kim[1], Tae-Hoon Kang[1],

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In this presentation, the manufacturing and microstructure, high-temperature tensile, creep, high-temperature fatigue and high-temperature oxidation properties of Ni based superalloys (IN625, IN718, IN738 etc.) have been suggested. In addition, the effect of heat treatment on the physical properties of each additively manufactured Ni-based superalloy has been also examined. Spherical powders for additive manufacturing manufactured by the gas atomizing process were used, and materials were manufactured using the L-PBF process under the optimal process conditions obtained through previous experiments for each alloy. The microstructure and physical properties of the obtained additively manufactured Ni-based superalloys were compared with those of the Ni-based superalloys manufactured by the conventional process, and through this, the characteristics of the Ni-based superalloys manufactured by the additive manufacturing process were confirmed and the deformation and fracture mechanisms thereof were identified. In addition, based on the advantages of reducing raw materials and improving physical properties through the realization of optimal shape design, the speaker would like to discuss the possibility of metal 3D printing as a manufacturing process of Ni based superalloys.

*Keywords: Ni-based Superalloy, Inconel alloys, Laser powder bed fusion, Microstructure, High temperature, Mechanical properties, Deformation behavior*

# In-situ synchrotron radiation X-ray diffraction study for understanding strengthening mechanisms of Al–Si alloy manufactured by laser powder bed fusion

**Naoki Takata[1],** Mulin Liu[1], Masahiro Hirata[2], Asuka Suzuki[1], Makoto Kobashi[1], Masaki Kato[3], Hiroki Adachi[2]

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## Abstract

In this study, the microstructural factors contributing to the high strength of additive-manufactured Al–Si alloys using laser powder bed fusion (L-PBF) were identified by in-situ synchrotron X-ray diffraction in tensile deformation and transmission electron microscopy. L-PBF and heat treatments were employed to manufacture Al–12%Si binary alloy specimens with different microstructures. At an early stage of deformation prior to macroscopic yielding, stress was dominantly partitioned into the α-Al matrix, rather than the Si phase in all specimens. Highly concentrated Si solute (~3%) in the α-Al matrix promoted the dynamic precipitation of nanoscale Si phase during loading, thereby increasing the yield strength. After macroscopic yielding, the partitioned stress in the Si phase monotonically increased in the strain-hardening regime with an increase in the dislocation density in the α-Al matrix. At a later stage of strain hardening, the flow curves of the partitioned stress in the Si phase yielded stress relaxation owing to plastic deformation. Therefore, Si-phase particles localized along the cell walls in the cellular-solidified microstructure of the L-PBF Al–Si alloys play a significant role in forming and increasing the number of dislocation obstacles, thereby enhancing strain hardening. This trend was observed in coarsened Si-phase particles in the cellular microstructure in the specimen heat-treated at 300 °C. In contrast, stress was slightly partitioned into a number of granular Si phases homogenously distributed in the α-Al matrix in the specimen heat-treated at a high temperature of 530 °C.

*Keywords: Laser powder bed fusion, Aluminum alloys, in-situ X-ray diffraction, Tensile deformation, Strain hardening*

# Balancing mechanical properties and deposition efficiency: the impact of oxidation in laser directed energy deposition

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Xiaoqi Chen[a], Guoxing Lu[a] and Shanqing Xu [a *]

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**Abstract:**

Oxidation is widely recognized as a key factor that affects the mechanical properties of materials in laser directed energy deposition (L-DED) process. However, it is found in this study that the oxidation also significantly impacts the deposition efficiency in L-DED process. Severe surface oxidation (oxygen content 2811 ppm) leads to significantly lower laser reflectance (14.5%), as compared with the absence of surface oxidation (71% laser reflectance with oxygen contents 229 ppm). Consequently, the melt pool temperature is found to be stabilised at 2300-2400 ℃ for severe oxidation and 1700-1800 ℃ for negligible oxidation, respectively. Moreover, the deposition efficiency of L-DED 316L process with severe oxidation exceeds that without evident oxidation by 1.7 times. Conversely, higher heat input and increased internal oxygen content (804 ppm) result in lower tensile properties for deposited 316L with severe oxidation (YS 456 MPa, UTS 631 MPa and elongation 57%), as compared with those without oxidation (YS 560 MPa, UTS 717 MPa, elongation 64%). This highlights the significant role of oxidation in creating a balance between deposition efficiency and mechanical properties of L-DED fabricated materials.

Key words: Laser directed energy deposition, oxidation, deposition efficiency, mechanical properties.

# The Effect of Grain Boundary Serration on Improving Hot Ductility of High Entropy Alloy Processed by Selective Laser Melting

**Meng-Yun Lee[1, 2, 3]**, Hyoung Seop Kim[2], An-Chou Yeh[1, 3]

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**Abstract**

$Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ high entropy alloy (Al02Ti03 HEA) is a kind of HEAs that contain FCC matrix and is mainly precipitation strengthened by $L1_2$ ($Ni_3Al$,Ti) phase. This HEA can successfully be manufactured by selective laser melting process, and posses excellent tensile performance at room temperature. However, with the increasing operation temperature, hot ductility drop occur at elevated temperature, and the crack propagation mainly starts from grain boundaries. Thus, grain boundary engineering has been conducted to generate serrated grain boundary in order to improve the hot ductility.

With the slow cooling rate of 1°C/min from the solution temperature to 900°C (SE treatment), the coarsened $L1_2$ phase could be generated at grain boundaries, and the grain boundary migration can be restricted during the heat treatment, resulting in the grain boundary serration. The aging process at 750°C for 50 hr is further conducted in order to form homogenous distribution of nano-sized $L1_2$ phase.

With grain boundary serration, the tensile ductility at 500°C can be improved from 12.83% to 16.28% in comparison with the heat treatment provided straight grain boundary morphology. Furthermore, as the testing temperature increases to 650°C, the elongation can be doubled and the ultimate tensile strength is also improved without significant compensation of yield strength. Thus, in this study, an effective method to improve the hot ductility of high entropy alloy is presented.

*Keywords: High entropy alloys, Grain boundary engineering*

# Creep and creep mechanism of electron beam-based powder bed fusion 316L stainless steel

**Kwang-Hyeok Lim**[1], Jong-Soo Bae[2], Xipeng Tan[3], and Gi-Dong Sim[4*]

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**Abstract**

Additive manufacturing is an emerging technology that enables the fabrication of net-shape complex structures and customized parts without any additional manufacturing process. In particular, a number of studies are focusing on the laser-based powder bed fusion (L-PBF) 316L stainless steel (SS) due to its superior strength without strength-ductility trade-off. However, the creep life of the L-PBF 316L SS are significantly lower than those of conventional 316L SS, which limits its applicability in nuclear power plants where creep resistance is crucial.

Here, we report the exceptional creep properties and mechanism of 316L SS fabricated by electron beam-based powder bed fusion (EB-PBF). Creep rupture time, creep rate, and creep exponent were obtained with custom-built high-temperature testing machine at 600 ℃ and 650 ℃. The creep life of EB-PBF 316L SS was 8 times higher than that of L-PBF 316L SS. In addition, the creep life of EB-PBF 316L SS was even 3 times higher than that of conventional 316L SS. The microstructure and elemental distribution were observed via X-ray diffraction (XRD), scanning electron microscope (SEM), electron backscattered diffraction (EBSD), and transmission electron microscope (TEM). Fine-sized C14 Laves phase (Fe2(Mo, Si)) and partially segregated Mo and Si were observed along the grain boundaries of samples tested at 600 ℃. In addition, coarsening of Laves phase precipitates was dominant adjacent to the silicon oxides ($MnSiO_3$) in the samples tested at 650 ℃. The possibility of formation of Laves phase during short term thermal exposure was demonstrated by thermodynamic calculations (JMATPRO). The exceptional creep properties are attributed to the early formation of fine C14 Laves phase along the grain boundaries which retards the grain boundary migration.

# Technical **Oral Session _ Session 1**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 1 (F1)** **10:50 - 12:10, Nov. 20**

**Chair :** Min Hyuk Park (Seoul National University), Cheng WANG (Tohoku University) 202A, 2F

10:50-11:20 **K-F0446** **[Keynote] Silica-based Hybrid Aerogel Films: Synthesis, Properties, and Application to Low Dielectrics**
Hyung-Ho Park (Yonsei University, Korea)

11:20-11:40 **I-F0807** **[Invited] Atomic layer deposition of two-dimensional materials**
Seong Keun Kim (Korea Institute of Science and Technology, Korea)

11:40-11:55 **O-F0716** **Microstructure and Properties of Diamond/Copper Composite by Supersonic Laser Deposition for Thermal Management**
Qunli Zhang (Zhejiang University of Technology, China)

11:55-12:10 **O-F0407** **Microstructure and mechanical properties of laser cladded WC-Co-Ni composite coatings for application to continuous caster roll**
Gibeom Kim (Pohang University of Science and Technology, Korea)

# Silica-based Hybrid Aerogel Films: Synthesis, Properties, and Application to Low Dielectrics

**Hyung-Ho Park**, Haryeong Choi, Taehee Kim

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**Abstract**

Aerogel refers to a material having a porous three-dimensional network structure composed of air in a high proportion of 90% or more. It is characterized by high porosity, small density (~3 mg/ml, three times of air) value and a high specific surface area (less than 1500 m2/g). At the same time, it has very low thermal conductivity (0.008 W/m/K), excellent sound insulation effect, and insulating properties with low dielectric constant (dielectric constant about 1.1). Through this, it is possible to control physical properties (hydrophobic, hydrophilic) and to provide additional functions. The unique and excellent physical properties of these aerogels are sufficient to have a variety of applications. The application fields of aerogel introduced in Fortune magazine are very diverse and extensive, with more than 800 types representing energy storage and saving materials, electrode materials for seawater desalination, ultra-low dielectric materials, and optical and acoustic materials. Although it is actively progressing, it is facing the limits of commercialization due to poor mechanical properties. In this presentation, the synthesis and characteristics of these aerogels will be examined, and among the research results for application in various fields of aerogels, research results related to the development of silica aerogels as semiconductor interlayer dielectric films will be introduced. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2020R1A5A1019131).

*Keywords: Silica aerogel; Hybrid; Ultra-low dielectric; High mechanical properties; Thin film*

# Atomic layer deposition of two-dimensional materials

**Seong Keun Kim**[1,2]

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**Abstract**

Two-dimensional (2D) metal dichalcogenides have drawn considerable interest because they offer possibilities for the implementation of emerging electronics. The emerging electronics are moving toward two major directions: vertical expansion of device space and flexibility. However, the development of a synthesis method for 2D metal dichalcogenides that meets all the requirements remains a significant challenge. In this talk, I will deliver the current status and limitations of atomic layer deposition of 2D semiconductors.

*Keywords: Two-dimensional materials, Atomic layer deposition, thin film transistors,*

# Microstructure and Properties of Diamond/Copper Composite by Supersonic Laser Deposition for Thermal Management

**Qunli Zhang**[1, 2, 3], **Yiyun Chen**[1, 2], **Bo Li**[1, 2, 3], **Jianhua Yao**[1, 2, 3]

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## Abstract

Diamond/copper composite has been considered as the exceptional thermal management material due to its excellent thermal conductivity. However, the natural unwettability between diamond and copper results in a large number of voids at the interface. Interfacial modification is an essential means of ameliorating interface bonding of diamond/copper composite. Supersonic laser deposition (SLD) is a hybrid process, which expands on the advantages of cold spray (CS), and realized high-rate deposition without melting, through locally heating the substrate at the deposition site by laser. In the present work, the diamond/copper composite was fabricated via SLD technology by adding metallization diamond into Cu powder as the feedstock. The results show that strong carbide metals made a well-arranged and uniformly distributed interfacial carbide layer in the interface region, which plays a critical role in increasing the amount of reactive interfacial bonding and decreasing defects. The diamond has not been abolished and graphitized but is strongly bonded with the Cu matrix due to the presence of carbide on surface of the diamond. The interface after laser irradiation can reduce the interfacial thermal resistance of the composites, thereby increase the thermal conductivity of the composites. Laser irradiation on the surface of the metallized diamond and copper substrate will enhance the contact area to form a thermal conductivity channel, which demonstrates that SLD technique is effective and potentially powerful to produce diamond/Cu composites for engineering applications.

*Keywords: Thermal management, diamond / copper composite, supersonic laser deposition, thermal conductivity.*

# Microstructure and mechanical properties of laser cladded WC-Co-Ni composite coatings for application to continuous caster roll

**Gibeom Kim[1]**, Jae-Eock Cho[1], Chang-Hee Yim[1], Yong-Chan Kim[2], Deok-Su Yun[3], Nam-Kyu Park[3], Rae-Hyung Chung[3], Dae-Geun Hong[1*]

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## Abstract

In the steel industry, foot rolls and support rolls are used to assist the initial solidification of slab exiting from the water-cooled copper mold in the primary cooling zone of continuous caster. These rolls are exposed to high stress and thermal cycling, which cause surface degradation and thermal cracking, and reduce their service life. Laser cladding can improve the mechanical properties and wear resistance of the coating layers of the rolls, but during the laser cladding process, the rapid temperature change and residual stress between coating layer and base material affect the mechanical properties and dimensional stability of the coating layer, and these problems could cause excessive heat-affected zones, cracks, and pore defects. Therefore, to improve the quality of the cladding layer, the applied cladding materials and process parameters must be optimized. This study investigated the effect of laser cladding process parameters on the microstructure and mechanical properties of WC-Co and WC-Ni composite coating. The cladding process was conducted with various laser powers, cladding speeds, and powder feeding rates. The phases, microstructure, and micro-hardness of the layer according to distance from the interface were analyzed in each specimen. In addition, WC-Co powders for increasing wear resistance and WC-Ni powders for increasing corrosion resistance were evaluated to determine their characteristics and applicability as cladding materials. The mechanical properties and tribological property of each powder with the same process parameter were compared and analyzed.

*Keywords: Laser cladding, WC composite coating, Microstructure, Hardness, Wear resistance*

## Acknowledgement

This work was supported by the Technology Innovation Program (20014733, Development of roll coating process and coating powder for fabrication of giga grade steel plate) funded By the Ministry of Trade, Industry & Energy (MOTIE, Korea).

# Technical **Oral Session _ Session 1**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 1 (G1)** **10:50 - 12:10, Nov. 20**

**Chair :** Young-Bum Chun (Korea Atomic Energy Research Institute) 303A, 3F

10:50-11:20 **K-G0242** **[Keynote] Development of Advanced Materials for Future Nuclear Systems**
Changheui Jang (Korea Advanced Institute of Science and Technology, Korea)

11:20-11:40 **I-G1112** **[Invited] Cr-coated accident tolerant nuclear fuel cladding and hydride embrittlement of Zirconium-based alloys: status, implications, and remaining challenges**
Youho Lee (Seoul National University, Korea)

11:40-11:55 **O-G0495** **Development of advanced neutron absorbing structural materials for spent nuclear fuel storage and transportation applications**
Young-Bum Chun (Korea Atomic Energy Research Institute, Korea)

11:55-12:10 **O-G0489** **Revealing the mechanism of irradiation-induced swelling in chromium through investigation of many types of defect structures**
Lijuan Cui (The University of Tokyo, Japan)

# Development of Advanced Materials for Future Nuclear Systems

**Changheui Jang[1],** Chaewon Kim[1], Hyun Joon Eom[1], Sumin Kim[1], Hyunmyung Kim[2], Ji Ho Shin[3], Gokul Obulan Subramanian[4]

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## Abstract

For the development of advanced nuclear systems like generation-IV reactors and fusion reactors, the requirement for the materials are ever demanding. Advanced nuclear systems generally operate at higher temperatures of 500 ~ 950 ºC, and structural materials are required to possess often combination of good strength and creep resistance, corrosion and oxidation resistance, and radiation resistance. Satisfying such properties, often in combination, poses quite a challenge for nuclear materials researchers. Nonetheless, there have been extensive advanced alloy development activity and some of the results are presented. First, alumina-forming duplex stainless steels (ADSS) were developed as accident tolerant fuel (ATF) cladding materials to replace the existing Zr-based alloys. ADSS showed excellent steam oxidation resistance with much higher strength than Zr-based alloys. Second, advanced radiation resistant stainless steels (ARES) were developed as structural materials for internals of light water reactors and blanket of fusion reactors. The excellent swelling resistance of ARES alloys were confirmed by heavy ion irradiation. Third, advanced creep enhanced stainless steels (ACES) were developed as structural materials for high temperature reactors. The excellent oxidation resistance and creep properties were confirmed in various environments. Finally, the development activity of innovative alloys for molten salt reactor (MSR), which requires highly corrosion resistant alloys with good creep properties, will be introduced.

*Keywords: Advanced nuclear systems, Creep resistance, Corrosion resistance, Irradiation resistance, Molten salt reactors*

# Cr-coated accident tolerant nuclear fuel cladding and hydride embrittlement of Zirconium-based alloys: status, implications, and remaining challenges

**Youho Lee[1],** Dongju Kim[1], HyunWoo Yook[1], Sunghoon Joung[1], Jinsu Kim[1], Dahyeon Woo[1], Chansoo Lee[1], Hyuntaek Rho[1], KyuSeok Sim[1], Changhyun Jo[1], Donghyeon Son[1], Boyeon Kwon[1], Jeonghyeon Lee[1], Wei Chen Low[1], Hyeongtak Kang[1]

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## Abstract

Coating a thin protective layer on Zirconium-based alloys for enhancing accident tolerance introduces changes in the overall nuclear fuel behaviour, including thermomechanical response, material embrittlement, and failure modes in both steady-state operation and accidents. Research is underway to explore the safety envelope and regulatory limits with integral fuel rod experiments, and modelling and simulation. The implications on the attainable performance gain with Cr-coated cladding are discussed, along with the key remaining challenges. In addition, recent progress in understanding the hydride embrittlement in Zirconium-based alloys with advanced characterization is discussed.

**Prof. Youho Lee** studies nuclear fuel materials, fuel performance modeling, and reactor safety and design. His research interests include accident tolerant fuel performance, nuclear fuel modelling and performance code development, spent fuel behavior with focus on hydride embrittlement, next generation nuclear fuel and reactor design, and nuclear construction process. Prof. Lee received a B.S. from the Korea Advanced Institute of Science and Technology (KAIST) in 2009, and an M.S. and Ph.D. in nuclear engineering from the Massachusetts Institute of Technology (MIT) in 2011 and 2013, respectively. He is currently an associate professor at the Department of Nuclear Engineering at Seoul National University (SNU). Prior to joining SNU, he served as an assistant professor at the University of New Mexico in the U.S.

*Keywords: Nuclear materials, Nuclear fuel, Zirconium-based alloys, Hydride embrittlement, Accident Tolerant Fuel (ATF)*

# Development of Advanced Neutron Absorbing Structural Materials for Spent Nuclear Fuel Storage and Transportation Applications

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## Abstract

Neutron absorbers used in spent nuclear fuel (SNF) storage systems including SNF racks and dry cask to control the criticality of SNF. Use of neutron absorber allows storage of SNF at maximum packing density and thereby providing certain economies of the SNF management. Al-$B_4C$ composites or cermets, which are most widely used neutron absorber, exhibit poor structural performance, especially low impact toughness and ductility, and accordingly SNF basket is fabricated in the form of triple-walled square tube consisting of two structural plates made of austenitic stainless steel and neutron absorber inserted in between. Neutron absorbing structural material, which can control criticality of SNF and structurally support SNF bundles at the same time, may turn bring considerable advantages including higher-density storage, simple and smaller basket, cheaper fabrication cost, and higher efficiency of heat dissipation, in the design and manufacture of SNF storage system. The present work introduces advance neutron absorbing structural material, which is based on new combination of matrix and neutron poisons, and show a possibility of design of single-walled basket in SNF dry storage system.

*Keywords: neutron absorber; spent nuclear fuel (SNF); criticality; structural integrity; toughness*

# Revealing the mechanism of irradiation-induced swelling in chromium - Through investigation of many types of defect structures

**Lijuan Cui**[1*], Yufeng Du[2], Huilong Yang[1], Sho Kano[1], Hiroaki Abe[1]

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**Abstract**

It has been revealed that compared with other bcc structural materials (Fe and W), Cr shows a significantly higher swelling rate at the initial irradiation stage, while much lower swelling at higher irradiation doses. Understanding the underground mechanism of this phenomenon is essential for the application of Cr-coatings in accident tolerance fuels. In the present study, pure chromium was irradiated by iron at swelling peak temperature of 550 ℃ to 0.1 and 15 dpa. The ratio of interstitial loops to vacancy loops is varied with irradiation dose. Special dislocation 'trough' and 'island' structures of a big outer dislocation loop and many small inner loops with inverse nature, were observed in the 0.1 dpa sample in certain crystal orientations. Such special structures have never been observed in other bcc materials. The distribution and evolution of dislocation defects, including loops, 'trough', 'island', and lines, revealed the mechanism of irradiation-induced swelling in Cr.

*Keywords: Accident tolerant fuel cladding, Dislocation loops, Irradiation, Chromium, Swelling*

# Technical **Oral Session _ Session 1**

## **Symposium H :** Electronic and Magnetic Materials

### Electronic and Magnetic Materials 1 (H1) — 10:50 - 12:20, Nov. 20

Chair : Jihoon Park (Korea Institute of Materials Sciences) — 303B, 3F

10:50-11:20 **K-H1111** **[Keynote] High-performance Nd-saving hot-deformed permanent magnets**
Jung-Goo Lee (Korea Institute of Materials Science, Korea)

11:20-11:40 **I-H1081** **[Invited] Synergistic effects of multiple elements in grain boundary diffusion Nd-Fe-B permanent magnet**
Lizhong Zhao (Hangzhou Dianzi University, China)

11:40-12:00 **I-H0174** **[Invited] Substitution and Phase Stabilization Elements Effects on Microstructure and Magnetic Properties of Sm-(Fe-Co) Based Magnets**
Jihoon Park (Korea Institute of Materials Sciences, Korea)

12:00-12:20 **I-H1177** **[Invited] Multidimensional understanding of the effect of iron content on iron-rich 2:17-type SmCo magnets: atomic occupancy, microstructure, and phase**
Tianli Zhang (Beihang University, China)

# High-performance Nd-saving hot-deformed permanent magnets

**Jung-Goo Lee[1],** Ga-Yeong Kim[2], Hee-Ryoung Cha[3], Tae-Hoon Kim[4]

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**Abstract**

Current challenge in Nd-Fe-B permanent magnets is to achieve high-performance Na-saving magnets. Nd is expensive and very unstable in supply and demand, but it is essential for realizing the high performance in rare earth permanent magnets. To realize the Nd-saving technology, the content of Nd should be reduced by replacing it with inexpensive Ce. However, until now, it has not been possible to prevent the deterioration of the magnetic properties of the magnet as the Ce content increases due to the inferior intrinsic magnetic properties of $Ce_2Fe_{14}B$ compared to $Nd_2Fe_{14}B$. In addition, it is recently reported that Ce-segregated $ReFe_2$ secondary phases are formed, which significantly deteriorate the microstructure and magnetic properties in the Nd-saving hot-deformed magnet. On the other hand, it has been reported that the deterioration of magnetic properties due to Ce substitution could be largely suppressed by developing a dual main phase structure in Nd-Fe-B sintered magnets. The short-range exchange coupling and long-range magnetostatic interaction induced by the peculiar chemical heterogeneity of dual main phase magnets are believed to be a key factor for improving coercivity and remanence of Nd-Ce-Fe-B sintered magnets. In this study, the limit of the hard magnetic properties of the Ce-substituted magnets was successfully surpassed by the hot-deformation using amorphous precursors that contain no (Nd, Ce)$Fe_2$ secondary phases. In addition, we also developed the dual main phase Nd-Ce-Fe-B hot-deformed magnets using two different amorphous melt-spun precursors with different compositions.

*Keywords:rare-earth magnets, Na-saving, amorphous, hot-deformation*

# Synergistic effects of multiple elements in grain boundary diffusion Nd-Fe-B permanent magnet

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## ABSTRACT

High performance Nd-Fe-B permanent magnet are key materials required in the fields of new energy, electronics industry and national defense industry. However, to high-power permanent magnetic motors, it is critical for Nd-Fe-B magnets to maintain the desirable coercivity at high-temperature operating conditions. To address this problem, two approaches, i.e. enhancing the room temperature coercivity and reducing the eddy current loss, are suggested in this work through the method of multi-rare earth synergistic grain boundary diffusion (GBD). First of all, the migration preferences of La, Ce, Pr, and Tb in the GBD process are investigated by first principles calculation. It is found that a higher diffusion depth of Tb elements and more homogeneous Tb-rich shells are achieved when La and Ce are introduced in the TbCu diffuser, which reduces the cost of diffuser and improves the magnetic performance at the same time. In addition, Pr with higher substitution energy was introduced into the TbAlCu diffuser, and it is found that Pr element prefers to segregate at grain boundaries during the diffusion process and leads to the formation of a large number of oxides with high resistivity in the grain boundary. Therefore, the resistivity of the $Tb_{35}Pr_{35}Al_{10}Cu_{20}$ diffused magnet is increased to $2.60\times10^{-6}$ Ωm, which is higher than that of $Tb_{70}Al_{10}Cu_{20}$ ($1.72\times10^{-6}$ Ωm). As a result, the simultaneous enhancement of the coercivity and resistance of the magnet could be successfully realized through the GBD process.

**Keywords:** Nd-Fe-B permanent magnet; grain boundary diffusion; Synergistic effects of multiple elements; coercivity; eddy current loss.

# Substitution and Phase Stabilization Elements Effects on Microstructure and Magnetic Properties of Sm-(Fe-Co) Based Magnets

**Jihoon Park[1]**, Tianhong Zhou[1] Chul-Jin Choi[1]

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## Abstract

$ThMn_{12}$-type structured magnetic material exhibits excellent magnetic properties surpassing those of rare-earth Nd-Fe-B magnets; the saturation magnetization, anisotropy field, and Curie temperature of the semiempirical data from Sm-Fe-Co thin film are 1.78 T, 12 T, and 859 K, respectively. However, its low intrinsic coercivity prohibited its usage as a permanent magnetic material. The magnetic properties of Sm-Fe-TM alloys, especially the intrinsic coercivity, are highly dependent on the nanostructure including grain size, intergranular phase thickness and material. Recently, Sm-Fe-TM sinter magnets with coercivity higher than 8 kOe have been fabricated by successfully controlling their grain boundary. However, their magnetizations must be increased to enhance maximum energy product. Therefore, in this work, we have studied Co substitution effects on the magnetization and minimized the intergranular phase to increase the magnetization and maximum energy product.

Sm-(Fe-Co)-based magnetic materials with additional Ti, V, and/or Cu-Ga were induction melted and homogenized at 1000 ºC. The resulting ingots were hydrogen decrepitated and jet-milled to micron-sized powders. The powders were then hot-pressed into green bodies, followed by sintering to produce bulk magnets. We found that not only the particle size of the jet-milled powder and the presence and thickness of intergranular phase affect the magnetization and coercivity, but also the Co concentration. Furthermore, the sintering condition are critical to maintaining the $ThMn_{12}$ phase and controlling nanostructure. The magnetic properties according to the initial composition, microstructure, such as grain size and grain boundary, etc. will be discussed in detail.

*Keywords: Permanent magnet, $ThMn_{12}$, grain boundary diffusion, coercivity, magnetization*

# Multidimensional understanding of the effect of iron content on iron-rich 2:17-type SmCo magnets: atomic occupancy, microstructure, and phase

**Tianli Zhang**, Mingyao Hu, Lei Yang, Longlong Xi, Dazhuang Kang, Bingjie Liu, Jun Cao, Cheng Xu, Shulan Zuo, Yangkun He, Chengbao Jiang

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**Abstract**

Iron-rich 2:17-type Sm-Co magnets are expected to possess a high energy product due to their elevated saturation magnetization. However, achieving high energy in manufactured magnets poses a challenge, and the mechanism by which the phases and microstructures are affected by the iron content remain unclear. Here, we investigate the phases and microstructures of 2:17-type Sm-Co magnets with varying iron contents in solid-solution precursors and aged magnets. Our study indicates that a higher iron content results in impure precursor by causing Sm-Co-Fe-Zr atomic occupancy competition. Increasing iron content also leads to microtwins with a lower dislocation density in the 1:7H precursor, resulting in an increased energy barrier and decreased driving force during the subsequent phase transformation. As a result, although iron-rich 1:7H single-phase precursor can be achieved by decreasing Sm and Zr content, the microtwins in precursor cause an increase of intermediate phases after decomposition. Furthermore, the impact of iron content on the 1:7H phase causes the aged magnets to have insufficient cell boundaries and massive grain boundary phases. Our study provides an understanding on the iron-rich 2:17-type Sm-Co magnets through the atomic, microstructural, and phase scales.

*Keywords: 2:17-type SmCo magnet, iron content, atomic occupancy, microstructure, phase structure*

# Technical **Oral Session _ Session 1**

## **Symposium I :** Biomaterials and Soft Materials and their Application

**Biomaterials and Soft Materials and their Application 1 (I1)** **10:50 - 12:30, Nov. 20**

**Chair :** Jongtaek Yeom (Korea Institute of Materials Science), Heungsoo SHIN (Hanyang University) 400, 4F

10:50-11:20 **K-I1161** **[Keynote] Ti-Nb based alloys with bone-like elastic modulus and large superelastic recovery strain**
Tae Hyeon Nam (Gyeongsang National University, Korea)

11:20-11:40 **I-I0494** **[Invited] Pulsed anodization to improve the biocompatibility of superelastic NiTi alloy**
Naofumi OHTSU (Kitami Institute of Technology, Japan)

11:40-12:00 **I-I0499** **[Invited] Development Status of Biocompatible Dental Ti-15Zr Alloy**
Nokeun PARK (Yeungnam University, Korea)

12:00-12:15 **O-I0219** **Evaluation of biological response to materials using intestinal epithelial cells and macrophages**
Tsuyoshi Kimura (Tokyo Medical and Dental University, Japan)

12:15-12:30 **O-I0831** **High strength and ductility in a bimodal grain structured biomedical Co–20Cr–15W–10Ni alloy for stent application**
Chenglin LI (Wuhan University, China)

# Ti-Nb based alloys with bone-like elastic modulus and large superelastic recovery strain

**Tae-hyun Nam**

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**Abstract**

Ti-Nb-Sn and Ti-Nb-Zr-Sn shape memory alloys were investigated to achieve the bone-like elastic modulus for biomedical applications by varying alloy compositions and thermos-mechnical treatment conditions to adjust the factors such as transformation temperature, β stability, ω phase amount and texture component which are well known to affect the elastic modulus of titanium alloys. The elastic modulus of 68.8 GPa in the Ti-15Nb-4Sn alloy decreased to 41.5 GPa in the 5Sn specimen due to the suppression of α" martensite, achieving the least β stability and the decrease in the amount of athermal ω (ωath) phase. A good combination of low elastic modulus and room temperature superelasticity was obtained in the 5Sn specimen. Significantly, a bone-like elastic modulus of 31.5 GPa is achieved in the 5.5Sn specimen, which has not been reported yet in titanium alloy sheets. In this specimen, (110) [001] (Goss texture) was developed as the dominant texture component and the ωath phase was completely suppressed. Also, the formation of the dominant Goss texture has not been reported previously in Ti–Nb–Sn alloy sheets. More detailly, along the rolling direction (RD), the [001]β//RD texture which effectively reduces elastic modulus along the RD was formed in 5Sn and 5.5Sn specimens and its intensity increased largely in the 5.5Sn specimen. Such a bone-like elastic modulus is attributed to the formation of a strong [001]β//RD texture as well as the absence of the ωath phase in β matrix.

*Keywords: Ti-Nb-Zr-Sn alloys, elastic modulus, superelasticity, texture, precipitates*

# Pulsed anodization to improve the biocompatibility of superelastic NiTi alloy

**Naofumi Ohtsu**[1], Ryota Kawakami[2], Yuya Matsui[3], Akihiro Tsuruta[4], Zi Wang[5], Makoto Ohta[6]

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**Abstract**

A fatal disadvantage of superelastic NiTi alloy when considering as biomaterial application is the Ni as the constituent element. Ni ion releases in the human body often induces cytotoxicity as well as allergic reaction, and medical doctors hesitate to use NiTi devices due to such risks. This presentation introduces a surface modification process that forms an almost Ni-free oxide layer improving the alloy's biocompatibility. The process is an electrochemical process being similar with anodization adopting a pulsed waveform voltage including voltage-off period. During the voltage-off period, anodic reaction is suspended but chemical reaction is highlighted, thereby enabling to remove Ni content from the alloy. As result, an oxide layer without Ni, corresponding to $TiO_2$, is formed on the alloy.

Actually, an almost Ni-free $TiO_2$ layer with a Ni content below a few percent was grown up to ~50 nm in thickness when anodized a NiTi alloy using a pulsed voltage in a nitric acid electrolyte. Such layer formation hydrophilized the surface, thereby activating cell extension and migration thereon. Also, forming surface region without Ni contributes the reduction of Ni ion release. As a result, cell proliferation rate on the pulsed-anodized NiTi alloy was superior to that on an untreated surface significantly.

The process does not raise the alloy's temperature; thus, metallographical change is negligible. The layer thickness is ultrathin; thus, the risk of peeling off is minimized. Based on above, the process is likely to be applicable as the industrial process.

*Keywords: NiTi alloy, Anodization, Hydrophilization, Removal of Ni, Cell activation*

# Development Status of Biocompatible Dental Ti-15Zr Alloy

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## Abstract

The aging population has led to a growing need for research and development of biomaterials for biomedical applications. Among them, implantable devices that directly interact with the human body require not only mechanical properties similar to those of living tissues but also biocompatibility without toxicity within the body. Titanium (Ti) and its alloys are suitable biomaterials as they form a durable titanium oxide layer on the surface, providing excellent corrosion resistance and high strength similar to bone. However, pure titanium has the disadvantage of relatively lower strength due to the lack of strengthening effects from alloying elements. The Ti-6Al-4V alloy, which contains aluminum (Al) and vanadium (V), has limitations as Al can induce Alzheimer's disease and V can cause cytotoxicity. For these reasons, recent research has focused on developing new materials that exhibit excellent biocompatibility and high strength. One notable example is the Ti-Zr binary alloy, where zirconium (Zr) is added to titanium. Zr has many similarities to Ti, making it a favorable choice for alloying. The addition of Zr not only enhances the mechanical properties but also makes it suitable as a biomaterial requiring high strength, thanks to its excellent biocompatibility. However, the development of Ti-Zr alloy faces various challenging situations from the perspectives of materials engineering and manufacturing processes. In our research laboratory, we aim to address these challenges by investigating the dissolution, solidification, heat treatment, sintering, and microstructure analysis through electron backscatter diffraction (EBSD), among other evaluations of the relationships between atoms. Through this symposium, we aim to share the current development status from various perspectives, ranging from thermodynamic and phase transformation aspects to practical applications, and engage in in-depth discussions based on this knowledge.

*Keywords: Titanium, Zirconium, dental implant, fabrication process, mechanical properties.*

# Evaluation of biological response to materials using intestinal epithelial cells and macrophages

**Tsuyoshi Kimura**[1], Chen Liang[2], Mika Suzuki[3], Yoshihide Hashimoto[4], Tadao Tanabe[5], Masaya Yamamoto[6], Akio Kishida[7]

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## Abstract

Investigating biological response to material is important to understand biocompatibility and cell-material interaction for biomaterial application. Macrophage is one of important cells for early biological response. In this study, we developed a pro-inflammatory evaluation method of material using a macrophage cell line (THP-1) tagged with luminescent peptide (HiBiT) genetically. Furthermore, epithelial cells (Caco-2) were co-cultured with the genome-edited THP-1 and the formation of tight junction between epithelial cells were investigated by transepithelial electrical resistance (TEER). The luminescent gene was inserted into IL-1β gene of THP-1 cell using CRISPR/Cas9 system. When the obtained HiBiT-tagged THP-1 cell was stimulated by LPS, the secretion of IL-1β was detected by luminescent measurement high-sensitively as well as ELISA and RT-PCR assays. Using the HiBiT-tagged THP-1 cell, it was founded that the production of IL-1β were differed between the used materials, PE, PP, cellulose and PTFE. Also, the different time course of the IL-1β secretion was observed between them. These results indicated the IL-1β production from the HiBiT-tagged THP-1 cell on the same sample could be measured over time. Furthermore, the resistance of Caco-2 co-cultured with the stimulated THP-1 was decreased for TEER measurement. From these results, we believe that the combination of pro-inflammatory measurement using the genetically engineered macrophage and TEER measurement of epithelial cell is useful for biological response to material.

*Keywords: Biological response, Macrophage, epithelial cell, genome-editing, tight junction*

# High strength and ductility in a bimodal grain structured biomedical Co–20Cr–15W–10Ni alloy for stent application

**Chenglin Li**[1], Jialin Guo[2] , Guodong Zhang[3]

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## Abstract

Co–Cr-based alloys have been extensively used as implant materials in dentistry, orthopaedics, and cardiology owing to their biological/mechanical compatibility and excellent corrosion resistance. Co–20Cr–15W–10Ni (L-605) is of particular interest for stent applications where high strength and ductility are important to enable thinner wall design and higher fatigue life and to improve stent deliverability and expandability. The strength–ductility of a metallic material strongly depends on the grain size and its distribution. Generally, a fine-grained structure enhances the strength by the Hall–Petch relation but limits the ductility, whereas a coarse-grained structure improves the ductility but reduces the strength. One effective approach for overcoming this strength–ductility trade-off is to produce heterogeneous structures. In this study, bimodal grain structures were tailored in Co–20Cr–15W–10Ni alloy via cold rolling followed by short-time annealing. The cold rolling induced a heterogeneous microstructure featuring the coexistence of severely and weakly deformed domains. During short-term annealing, fine and coarse grains were preferentially recrystallized in severely deformed regions and weakly deformed domains, respectively, resulting in a bimodal grain structure consisted of fine grains (~1–2 μm) and coarse grains (~10–20 μm). The bimodal structure provided a well-balanced strength–ductility with an ultimate tensile strength of 1200-1300 MPa, a low yield strength of 500-700 MPa, and a high ductility of ~50-60%, making that suitable for stent applications.

*Keywords: Biomaterials; L605 alloy; bimodal structure; high strength and ductility; stent.*

# Technical **Oral Session _ Session 1**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 1** **10:50 - 12:25, Nov. 20**

Chair : Michael Preuss (Monash University) 201B, 2F

10:50-11:20 **I-J0482** **[Keynote] Effect of Heterogeneous Deformation Microstructure on the Primary Recrystallization Behavior of FCC Alloys**
Shi-Hoon Choi (Sunchon National University, Korea)

11:20-11:40 **I-J0567** **[Invited] Structure, interfacial segregation and transformations of precipitates in lightweight alloys**
Laure Bourgeois (Monash University, Australia)

11:40-11:55 **O-J0711** **High-throughput phase diagram examinations on multicomponent systems using sintered diffusion multiples**
Teruyuki Ikeda (Ibaraki University, Japan)

11:55-12:10 **O-J1001** **Evolution of the Microstructural Parameters and Twining Behavior in 316L Stainless Steel during Deformation Process by in-situ EBSD**
Bin Huang (Northwestern Polytechnical Unversity, China)

12:10-12:25 **O-J0914** **Micromechanical properties of Cu micro-lattice under extreme deformation conditions**
Kang Sung-Gyu (Max-Planck-Institut Für Eisenforschung, Germany)

# Effect of Heterogeneous Deformation Microstructure on the Primary Recrystallization Behavior of FCC Alloys

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## Abstract

The stacking fault energy (SFE) of FCC alloys is a critical parameter that influences the microstructure and texture evolution during deformation and annealing treatments. Inhomogeneous plastic deformation could lead to the heterogeneities in the recrystallization phenomena. The evolution of the mechanical twins, shear bands (SBs)/strain localizations (SLs), and strain induced martensite (SIM) in FCC alloys can cause heterogenous deformation behavior. Recrystallization kinetics depend on the amount of internal stored energy (SE) accumulated during deformation as well as the recrystallization temperature and time. This study investigated the impact of deformed microstructure on the annealing behavior of aluminum (Al-1wt.%Mg and AA1100), copper (Cu-Fe-P), and Cantor (i.e., equiatomic CoCrFeMnNi HEA) alloys, which exhibits varying SFEs. All alloys were cold-rolled to an 80% thickness reduction and annealed at different temperature. Primary recrystallization for Cu-Fe-P was observed at room temperature (RT), known as self-annealing, where the nucleated grains were observed at the SLs as well as deformed GBs. Al-1wt.%Mg sheets were subjected to symmetric rolling (SR) and asymmetric rolling (AR) followed by heat-treatment at 350-450°C for different time intervals. Variation in recrystallization kinetics was observed for SR and AR, while deformed AA1100 showed dependency of recrystallization behavior on the initial grain size. Cantor alloy (80% rolled) was subjected to annealing treatment at 700°C for different time interval (5 min –1 hr). The evolution of multiple annealing twins and their effect on the texture was discussed for the heat-treated Cantor alloy. This study comprehensively reports the impact of heterogenous deformation on primary recrystallized microstructure and crystallographic texture evolution of the given FCC materials using results from electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), and X-ray diffraction (XRD).

***Keyword:*** *Heterogenous Deformation, Primary Recrystallization, Shear Band, Crystallographic Texture, Stored Energy.*

# Structure, interfacial segregation and transformations of precipitates in lightweight alloys

**Laure Bourgeois**[1], Shenghan Su[2], Zezhong Zhang[3] and Nikhil V. Medhekar[4]

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## Abstract

Solid-state precipitates are key components of many materials, and none more so perhaps than of lightweight alloys such as aluminium. These precipitates are often deeply buried inside the alloy matrix due to having at least one dimension at the nanoscale or even sub-nanoscale. These precipitates are also, in most cases, metastable phases that do not exist in a monolithic state, thus constituting difficult objects to characterise at the atomic scale.

In this contribution we present the structural determination of several precipitate phases in lightweight alloys, including the well-known Al-Cu, Al-Au and Al-Ag systems. Using a combination of in-situ heating in the transmission electron microscope (TEM) and atomistic simulations, we reveal not only the existence of new interfacial structures and precipitate phases, but also their mechanisms of transformation. This includes new pathways to the formation of desired strengthening precipitates. These insights are used as a starting point to predict the precipitation behaviour of other, largely unexplored, alloy systems.
The challenges and advantages of atomic-scale characterisation of buried nanoprecipitates using aberration-corrected TEM and *in-situ* heating in the TEM are discussed.

*Keywords: atomic-scale structure; aluminium alloys; transmission electron microscopy; atomistic simulations*

# High-throughput phase diagram examinations on multicomponent systems using sintered diffusion multiples

**Teruyuki Ikeda**[1], Ryuta Yurishima[2], Ayako Ikeda[3]

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**Abstract**

Enhancements of material functions or discoveries of novel materials with high performance are often accompanied with increase in number of constituent elements. Thus, investigations on multicomponent systems have attracted growing attention. However, the increase in number of components imposes great increase in number of samples required to construct phase diagrams if a conventional way of experiments, where samples are prepared one by one, are taken. Therefore, it is necessary to develop a new strategy to accelerate surveys of phase diagrams of multicomponent systems.

In this study, we propose an experimental route for examining phase diagrams and hence searching for unknown phases in multicomponent systems using sintered diffusion multiples ("SDMs"). Diffusion multiple samples with 3 to 5 constituent elements were prepared by sintering elemental powder mixture and diffusion annealing. After annealing, chemical compositions in the samples were analysed at random by a point analysis mode of electron probe micro analysis.

As results of the analyses, in principle, the plots of all experimental chemical compositions in a compositional space contain information on the existence ranges of existing phases. Therefore, careful analysis of the plots yields phase diagrams. In this study, we have developed the method of analysis to obtain phase diagrams, that is, phase boundaries and tie lines, from experimental data from SDM approaches. We also discuss how to evaluate the validity of the phase diagrams determined in this way.

*Keywords: sintered diffusion multiples, high-throughput studies, multicomponent phase diagrams*

# Evolution of the Microstructural Parameters and Twining Behavior in 316L Stainless Steel during Deformation Process by in-situ EBSD

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**Abstract**

The evolution of the microstructural parameters and twinning behavior in 316L stainless steel during deformation process is of great significance for understanding its deformation mechanism. In this work, in-situ electron backscatter diffraction (in-situ EBSD) were used to study the microstructural parameters and twinning behavior in 316L stainless steel during tensile process. With the increase of deformation, the grain orientation in 316L stainless steel gradually shifts from <101> paralleling to the tensile direction to <111> paralleling to the tensile direction, as well as the average Schmid factor decreases and the orientation becomes harder. The large angle grain boundaries (HAGB) and twining boundaries hinder the movement of dislocations, causing the value of Kernel average misorientation (KAM) near the grain boundaries increases with increasing of deformation. The deformation twinning tends to occur in the matrix with harder orientation and annealing twinning. The deformation twinning occurs dramatically in grains with<111>//RD orientation and partially in grains with<101> //RD orientation but in grains with<001>//RD orientation. For the grains that contain annealing twinning initially, when the angle between the annealing twinning boundary and the tensile direction falls into the range of 10-20 ° and 60-80 °, deformation twinning formed easily during the tensile process. When the grains with a small size and a large number of annealing twinning boundaries, deformation twinning tends to be appeared in the matrix because the annealing twinning boundaries can impede the plastic deformation.

*Keywords: 316L stainless steel, in-situ EBSD, deformation twining, annealing twining, tensile process*

# Micromechanical properties of Cu micro-lattice under extreme deformation conditions

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## Abstract

Lattice structures with interconnected 3D solid frames and open pore channels are promising structural materials for challenging environments due to their exceptional strength and ability to absorb energy during deformation. Enhancing the mechanical performance of lattice structures can be achieved by leveraging the "smaller is stronger" size effect. However, conventional microfabrication techniques like UV lithography are limited to 2.5D geometries, making it impossible to fabricate intricate structures such as microlattices. In this research, we introduce a novel additive micromanufacturing process based on localized electrodeposition to produce metal microlattices. We specifically focus on fabricating pure copper microlattices and investigate their structure, microstructure, and mechanical properties. NanoCT imaging confirms the microlattices possess a well-defined structure with excellent connectivity between nodes and struts. Electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM) analyses reveal that the microlattices exhibit an ultrafine-grained structure with a significant presence of nanotwin boundaries. Subsequently, we assess the mechanical properties of the copper microlattices across a wide range of strain rates (0.001/s to 100/s) and at varying temperatures (-150 and 25 °C) using an *in situ* SEM micromechanical testing setup based on piezoactuator. This study demonstrates the successful fabrication of complex 3D metal architectures at the micron scale, which exhibit exceptional mechanical properties suitable for demanding dynamic and extreme loading conditions.

*Keywords: Microlattice, Mechanical properties, in situ mechanical testing, extreme deformation conditions*

# Technical **Oral Session _ Session 1**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 1** **10:30 - 12:30, Nov. 20**

**Chair :** En MA (Xi'an Jiaotong University) Samda Hall B, 3F

10:50-11:20 **K-K0493** **[Keynote] Favourable strengthening mechanism in CrCoNi medium entropy alloy: an in situ neutron diffraction study**
Wan Chuck WOO (Korea Atomic Energy Research Institute, Korea)

11:20-11:40 **I-K0780** **[Invited] A new approach to quantify short-range ordering (SRO) using atom probe tomography (APT) in CoCrNi alloys**
Mengwei He (The University of Sydney, Australia)

11:40-12:00 **I-K1027** **[Invited] Long-Tail Effect Combined High-Throughput Design of Cu-based High-entropy Alloys**
Yong ZHANG (University of Science and Technology Beijing, China)

12:00-12:15 **O-K0866** **Bulk and grain boundary tracer diffusion in multiphase AlCoCrFeNiTi0.2 compositionally complex alloy**
Ruixuan Li (University of Science and Technology Beijing, China)

12:15-12:30 **O-K0738** **A novel methodology to estimate hydrogen diffusivity and its applications in revealing hydrogen effects in CoCrNi medium-entropy alloy versus 316L stainless steel**
Dong-Hyun Lee (Chungnam National University, Korea)

# Favourable strengthening mechanism in CrCoNi medium entropy alloy: an in situ neutron diffraction study

**Wanchuck Woo**[1], Hobyung Chae[1], Soo Yeol Lee[2], YoungSang Na[3], Stefanus Harjo[4], Ke An[5]

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**Abstract**

Strengthening via dislocation slip and deformation twinning was compared between cast-wrought (CW) and additively manufactured (AM) equiatomic CoCrNi medium-entropy alloys (MEAs). In situ neutron diffraction experiments and line profile analyses correlated the faulting-embedded crystal structure to the dislocation density, stacking/twin fault probability, and stacking fault energy as a function of strain. The results show that the dislocation density of $7.2 \times 10^{14}$ $m^{-2}$ in CW and $1.7 \times 10^{15}$ $m^{-2}$ in AM at the strain of 0.45. Those dislocation densities contributed to the flow stress of about 470 MPa in CW and 600 MPa in AM, respectively. Meanwhile, the twin fault probability of CW (2.7%) was about two times higher than AM (1.3%) near fracture. The twinning can provide the strengthening of 360 MPa in CW and 180 MPa in AM. Consequently, it suggests that the favourable strengthening mechanism is twinning in CW and dislocation slip in AM. The strengthening behaviour can be attributed to the stacking fault energy. It was estimated as 18.6 $mJ/m^2$ in CW and 37.5 $mJ/m^2$ in AM MEAs analysed by the strain field of dislocations incorporated model. Dense dislocations, deformation twinning, and atomic-scale stacking structure were examined by using electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM).

*Keywords: dislocation density, twinning, neutron diffraction, strengthening, CrCoNi medium-entropy alloy.*

# A new approach to quantify short-range ordering (SRO) using atom probe tomography (APT) in CoCrNi alloys

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## Abstract

Medium entropy alloys (MEAs) are currently attracting enormous scientific interest due to their exceptional combination of strength and ductility. However, the potential for and causality of SRO behaviour in these alloys have sparked considerable debate. While some researchers found a strong positive correlation between SRO behaviour and mechanical properties such as yield strength. Others contend that the influence of SRO in the alloy is negligible. This discrepancy even arises within similar systems subject to different heat treatment conditions.

To address this debate, precise quantification of SRO parameter under various heat treatments conditions becomes imperative. In this study, we propose a novel approach utilizing APT for accurate SRO quantification. Significantly, this resolves the contentious issue and provides a comprehensive calculation framework to determine the feasibility of SRO measurement using an atom probe microscope, considering the instrumental performance and alloy composition.

We conducted a series of simulations to establish direct relationships between the diminishment of SRO values with APT detection efficiency, and spatial noise. This enabled us to determine the thresholds where SRO quantification is achievable. Moreover, for cases where SRO measurements are plausible, the simulations yielded correction factors that could be applied to SRO values determined from raw experimental APT data to reconstitute the true values. To validate our methodology, we applied the simulation pipeline and correction factors to CoCrNi MEAs with a coarse-grained microstructure subjected to diverse thermal processing. Notably, discrete variations in SRO behaviour were observed.

Based on our current findings, more accurate modelling of the atomic structure can be achieved. Consequently, it presents a compelling opportunity to comprehend the microstructural mechanisms that govern mechanical property performance at the atomic scale.

*Keywords: high entropy alloy; short range ordering; atomic clustering; atom probe tomography; microscopy.*

# Long_tail Effect Combined High-Throughput Design of Cu-based High-entropy Alloys

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**Abstract**

Although equi atomic ratio is preferred for the high entropy alloys, we also obtained excellent properties by Combined Al with a four-elements alloys, MgZnCuLi, which is forming high-entropy Al. Many alloys composition with 80_20% showing excellent properties, e.g., Al80(MgZnCuLi)20 showing 800 MPa compressive strength; Fe80B20, with very nice glass forming ability and magnetic properties; The 80_20% rule is also familiar as long_tail effect. The long_tail is a statistical pattern of distribution that occurs when a larger share of occurrences occur farther away from the centre or head of distribution. This means that a long tail distribution includes many values that are far away from the mean value. In an economic context, this signifies that more products are purchased that are different from the most mainstream products. The paper will verify that in a CuCoCrFeNi alloy system, by the high-throughput_technology, that long_tail effect also work. The microstructures, mechanical behaviors, and electrical conductivity of the Cu80(CoCrFeNi)20 alloys were systematically studied, the alloy has been named as high-entropy Copper.

*Keywords: High entropy alloys; long-tail effect; high-throughput technology; Cu based Alloys; Electrical Conductivity; mehcanical behavior.*

# Bulk and grain boundary tracer diffusion in multiphase AlCoCrFeNiTi0.2 compositionally complex alloy

**Ruixuan Li[1,2],** Gerhard Wilde[2], Yong Zhang[1], Sergiy V. Divinski[2]

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**Abstract**

Atomic self-diffusion and interdiffusion have been studied extensively in single-phase high entropy alloys (HEAs) because of their earliest claimed sluggish diffusion effect, which is closely related to the phase stability, precipitation transformation, mechanical behaviours, etc. Different phase structures, such as the face-centered cubic, body-centered cubic, and hexagonal close-packed structures, have been studied, and only the sluggish diffusion of the face-centered-cubic HEAs has been unanimously recognized.

To the best of our knowledge, there are no reports on diffusion studies in multi-phase compositional complex alloys (CCAs) and especially along the interphase boundaries. Such diffusion behaviour is hardly being accessible via a conventional diffusion couple technique. Therefore, it is extremely important to quantify the diffusion rates in the multiphase CCAs through direct self-diffusion measurements using a tracer approach.

In this study, the near-equiatomic AlCoCrFeNiTi0.2 CCA is chosen as the target. Tracer self-diffusion of Co in a compositionally complex AlCoCrFeNiTi0.2 alloy is measured using the radiotracer technique. The complex multi-phase microstructure (a mixture of BCC, B2, σ, and FCC phases in dependence of the processing conditions) is carefully analyzed to quantify the measured concentration-depth profiles in terms of volume and short-circuit diffusion contributions. The analysis allowed to determine the volume diffusion coefficients in the B2 phase and those along the high-angle B2/B2 grain boundaries (GBs). The absence of any "sluggishness" of diffusion in this alloy is unambiguously verified, both for volume and GB diffusion contributions.

*Keywords: High-entropy alloys, Compositionally complex alloys, Diffusion, Grain boundary, Interphase boundary*

# A novel methodology to estimate hydrogen diffusivity and its applications in revealing hydrogen effects in CoCrNi medium-entropy alloy versus 316L stainless steel

**Dong-Hyun Lee**[1], Yun Hee An[1], Yakai Zhao[2], Ju Hyeok Lee[1], Hyun You Kim[1], You Sub Kim[1], Soo Yeol Lee[1]

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**Abstract**

Hydrogen diffusivity is one of the important factors affecting the susceptibility to hydrogen embrittlement of metals and alloys. Here, we proposed a novel approach to estimate hydrogen diffusivity in FCC alloys by performing nanoindentation experiments with continuous stiffness measurement. In consideration of the plastic zone size around the indentation, the relationship between hydrogen-induced hardness change and the depth from the sample surface was established for two typical FCC alloys—316L stainless steel (SS) and CoCrNi medium-entropy alloy (MEA)—subjected to hydrogen-charging and subsequent room-temperature aging. By combining with the estimation of the through-thickness distribution of hydrogen concentration, hydrogen diffusivity values were successfully determined, which agreed well with the literature data. It was revealed that CoCrNi MEA exhibited a hydrogen diffusivity ~0.7 times higher than that in SS316L, and that hydrogen-induced softening upon long-term aging (at room temperature) was observed in CoCrNi but not in SS316L. The underlying mechanisms for the distinct hydrogen-related phenomena in CoCrNi MEA were elucidated based on the density functional theory calculations of hydrogen solution energy and vacancy formation energy.

*Keywords: nanoindentation; hardness; hydrogen diffusivity; face-centered cubic; stainless steel; medium-entropy alloy.*

# Technical **Oral Session _ Session 1**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 1 (L1)** **10:50 - 12:25, Nov. 20**

Chair : Hisashi Sato (Nagoya Institute of Technology), Seungchan Cho (Korea Institute of Materials Science) 202B, 2F

10:50-11:20 **K-L0353** **[Keynote] Functionally graded carbon nanotube-reinforced aluminium matrix composites for air conditioning and heating application of electric vehicles**
Hansang Kwon (Pukyong National University, Korea)

11:20-11:40 **I-L0133** **[Invited] Fabrication of ceramic particulate reinforced metal matrix composites using casting process**
Seungchan Cho (Korea Institute of Materials Science, Korea)

11:40-11:55 **O-L0347** **Fabrication of dispersion strengthened Al-Y2O3 with bimodal grain size distribution via powder metallurgical route**
Tatsuaki Sakamoto (Ehime University, Japan)

11:55-12:10 **O-L0839** **High-performance titanium matrix composites fabricated by hot isostatic pressing**
Shuai Wang (Harbin Institute of Technology, China)

12:10-12:25 **O-L0749** **Microstructural and dry sliding wear behavior of particulate reinforced copper matrix composites fabricated by in situ casting process**
Cunlei Zou (Dalian Jiaotong University, China)

| K-L0353 |

# Functionally graded carbon nanotube-reinforced aluminium matrix composites for air conditioning and heating application of electric vehicles

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## Abstract

Thermal management material is one of the essential components of electric vehicles (EVs), such as batteries and motors. Significantly, high thermal conductive materials affect the EV's air conditioning and heating system efficiency. For example, suppose the component materials are not delivering the heating and cooling well. In that case, the battery consumption is significantly increased because an electrical power system runs all of the electronic devices, including air conditioning and heating of the EV.

In this study, we focused on developing high thermal conductive pipe materials with tailoring properties based on the concept of the functionally graded material. The functionally graded composite materials were prepared through a hot-extrusion process, and the carbon nanotubes were utilized as reinforcing material in the aluminium matrix.

**Keywords:** Aluminium, Carbon Nanotubes, Functionally Graded Materials (FGM), Extrusion.

# Fabrication of ceramic particulate reinforced metal matrix composites using casting process

**Seungchan Cho[1],** Junnghwan Kim[1], Donghyun Lee[1], Sangmin Shin[1], Sang-Bok Lee[1], Sang-Kwan Lee[1]

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**Abstract**

In order to facilitate the development of crucial infrastructure industries, such as automobiles, aircraft, transportation equipment, and power plants, there is an increasing demand for materials that can substantially reduce weight and enhance properties compared to traditional metals. Metal matrix composites (MMCs) have captured the attention of both scientific and industrial communities due to their tailored characteristics, which provide unique structural and functional properties that cannot be achieved in monolithic metal structures. A promising approach for enhancing mechanical and physical properties, including strength, elastic modulus, hardness, and coefficient of thermal expansion (CTE), while achieving substantial weight reduction beyond what can be accomplished through alloy design, involves the addition of ceramic reinforcements such as titanium carbide (TiC), boron carbide ($B_4C$), and silicon carbide (SiC) to a metal matrix. In this study, we utilized various casting processes to fabricate uniformly dispersed, high-volume fraction ceramic particulate reinforced MMCs.

*Keywords: Metal matrix composite, ceramic reinforcement, casting.*

# Fabrication of dispersion strengthened Al-$Y_2O_3$ with bimodal grain size distribution via powder metallurgical route

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## Abstract

We fabricated dispersion strengthened Al-$Y_2O_3$ with the Al matrix grain size in a bimodal distribution for enhancement of strength-ductility combination. Al-4wt%$Y_2O_3$ was prepared by mechanical alloying (MA). The MA powder of Al-4wt%$Y_2O_3$ and pure Al powder were blended and consolidated by spark plasma sintering (SPS). The consolidated compact exhibited a bimodal grain size distribution of the Al matrix. Transmission electron microscope (TEM) observation showed that the coarse (about 2 μm) and fine grains (about 300 nm) were derived from the Al and MA powders, respectively. For comparison, specimens with a unimodal grain size distribution were also prepared by consolidating the pure Al and the MA powder separately. Yield strengths and uniform elongations were evaluated by tensile test. The strength-ductility balance of the bimodal specimen is not so good as compared to the unimodal specimens. However, the strength-ductility balance was improved by short-time mechanically milling (40 min) of blended powder of pure Al and the MA powders before SPS. This enhancement was attributed to the increase in the interface between the coarse and fine grains, leading to the introduction of geometrically necessary dislocations. Consequently, dislocation density was likely to increase during deformation, and the strain hardening rate was increased, resulting in the enhancement of uniform elongation.

*Keywords: Strength-ductility combination, Heterogeneous nanostructure, Mechanical alloying, Geometrically necessary dislocation, Strain hardening rate*

# High-performance titanium matrix composites fabricated by hot isostatic pressing

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## Abstract

Titanium matrix composites (TMCs) can be used as structural materials in the aerospace field due to their good high-temperature performance and low density. However, the processing of TMCs is difficult, the price is high, and thus the use is hindered. Hot isostatic pressing (HIP), as an advanced material fabrication method, can achieve the fabrication and formation of the material simultaneously. The material utilization ratio can also be significantly improved. Therefore, HIP is a very suitable method for the fabrication of TMCs. It is common to use steel capsules in this process. But for TMCs, the contradiction is: eutectic reactions between iron and titanium occur at 1080 ℃. But the in-situ reaction temperature of the TiB reinforcement phase exceeds 1100 ℃. To avoid this contradiction, we brought up a novel two-step strategy for HIP of TMCs. It has been found that compared with the TMCs fabricated by the normal process, the TMCs herein fabricated by the new HIP strategy exhibited 100 MPa incensement in the room temperature strength, and the high temperature (650-700 ℃) strength was also increased by 50 MPa. It is believed that the formation of nano-scale TiB reinforcement and the two-modal titanium matrix grain structure contributed to the strength enhancement.

*Keywords: titanium matrix composites; hot isostatic pressing; mechanical properties; strength-ductility enhancement*

# Microstructural and dry sliding wear behavior of particulate reinforced copper matrix composites fabricated by in situ casting proces

**Cunlei Zou**[1], Chuang Dong[1,2]

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## Abstract

Particulate reinforced copper matrix composites $TiB_2$ particles reinforced copper matrix composites were fabricated by traditional casting from in-situ synthesized between Cu-B and Cu-Ti master alloy. The microstructure and mechanical properties of the composites with different content of $TiB_2$ and loading wear condition on the tribological behavior of Cu/$TiB_2$ composites were investigated. The results show that $TiB_2$ particles are in situ formed in the copper matrix and the TEM images show the well bonding between copper and $TiB_2$. With the increasing amount of in-situ $TiB_2$ particles in copper matrix, the tensile strength and hardness are significantly improved, but the elongation and electrical conductivity slightly decrease. The friction and wear characteristics of the composites have been determined by carrying out dry sliding tests on pin-on-disk machine under different loads, speed and time. The volume loss rate of the composites under different condition shows the significant improvement of wear property with the addition of $TiB_2$ particles in copper matrix.

*Keywords: In situ copper matrix composite, Microstructure, Wear, Mechanical properties.*

# Technical **Oral Session _ Session 1**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 1 (M1)** **10:50 - 12:30, Nov. 20**

**Chair :** Yoon Suk Choi (Pusan National University) 402, 4F

10:50-11:20 **K-M1085** **[Keynote] Heterostructured Materials: A Fast-Developing New Materials Field**
Yuntian Zhu (City University of Hong Kong, China)

11:20-11:40 **I-M0781** **[Invited] Ligament size effect in creep of nanoporous gold**
Ju-Young Kim (Ulsan National Institute of Science and Technology, Korea)

11:40-12:00 **I-M1073** **[Invited] Novel properties of plasmonic metal nanostructures for sensing and cancer therapy: a case study of hollow gold nanospheres**
Jin Zhang (University Of California Santa Cruz, USA)

12:00-12:15 **O-M0565** **Ultra-high strength and ductility of a multiple component alloy with heterogeneous grains and precipitates**
Yong Zhang (Nanjing University of Science And Technology, China)

12:15-12:30 **O-M1155** **Polymer Alloying by Severe Plastic Deformation (SPD) - New Potential of Producing Materials with Exceptional Properties**
Yajun ZHAO (Dalian Jiaotong University, China)

# Heterostructured Materials: A Fast-Developing New Materials Field

**Yuntian Zhu,**

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## Abstract

Strong and tough materials are desired for energy-efficient applications such as electric cars and aerospace applications. Recently, heterostructures are found to produce unprecedented strength and ductility that are considered impossible from our textbook knowledge and materials history. Heterostructured materials consist of heterogeneous zones with dramatic (>100%) variations in mechanical and/or physical properties. The interaction in these hetero-zones produces a synergistic effect where the integrated property exceeds the prediction by the rule-of-mixtures. Importantly, HS materials can be produced by current industrial facilities at large scale and low cost. There are many scientific issues with such materials that challenge the communities of experimental materials science and computational material mechanics. Heterostructured materials is quickly becoming a hot research field with multiple international conferences/workshops organized in different countries per year. In this talk I'll present the progress in heterostructured materials as well as future challenges and issues.

*Keywords: Heterostructured materials, Hetero deformation induced (HDI) stress, Geometrically necessary dislocations, Strain gradient, Strain partioning*

# Ligament size effect in creep of nanoporous gold

**Ju-Young Kim[1]**

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## Abstract

Spherical nanoindentation creep tests were performed on four nanoporous gold samples, each having ligament sizes of 30 nm, 103 nm, 417 nm, and 986 nm. Our investigation reveals that creep behavior is influenced by the size of the ligaments, with a noticeable increase in both total creep strain and creep strain rate as the ligament size increases within the range of 103 nm to 986 nm. Interestingly, the most pronounced creep is observed in the sample with a ligament size of 30 nm. To further explore the effects of surface coating, a 2-nm-thick alumina layer was applied to the ligaments. It was observed that the creep behavior increased for ligament sizes ranging from 103 nm to 986 nm when coated with alumina. Conversely, for the ligament size of 30 nm, the surface coating resulted in a decrease in creep. The ligament-size dependent creep phenomenon and the influence of surface coating are discussed in relation to the dominant dislocation mechanism occurring within the ligaments during dislocation-mediated creep for each specific ligament size.

*Keywords: Nanoporous gold, indentation size effect, in-situ nano-mechanical testing, self-similarity, microstructure*

# Novel properties of plasmonic metal nanostructures for sensing and cancer therapy: a case study of hollow gold nanospheres

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Nanomaterials of metal have novel properties and useful functionalities. As an important member of the family of plasmonic metal nanostructures, hollow gold nanospheres (HGNs) exhibit unique optical and photothermal properties desirable for many applications including SERS (surface enhanced Raman scattering) sensing, optical imaging, drug delivery, and photothermal therapy (PTT) of cancer. We have conducted extensive studies of the mechanism behind the growth of HGNs and determined the important role several factors including oxygen in the reaction process using a number of spectroscopic techniques including X-ray spectroscopy. Based on the better understanding of the growth mechanism, we are able to control the synthesis of HGNs with well-defined size and shell thick, allowing surface plasmon resonance (SPR) at specific wavelength to be achieved, especially the highly desired near IR (NIR) region of strong interest for biomedical applications. We also control the surface morphology of the HGNs by varying surface ligand molecules. The synthesized HGNs have been used for *in vitro* studies of HGN-mediated PTT of oral squamous cell carcinoma. Furthermore, we have synthesized hollow gold nanostars and Ag-coated hollow gold nanostars with improved SERS activity due to creation of hot spots on the HGN surface.

*Keywords: optical property, plasmonics, hollow gold nanospheres (HGNs), photothermal ablation therapy; surface-enhanced Raman scattering (SERS).*

# Ultra-high strength and ductility of a multiple component alloy with heterogeneous grains and precipitates

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**Abstract**

In the present study, a heterogeneous microstructure characterized by a mixture of nano-grains and ultrafine-grains embedded with γ' precipitates is fabricated by cold rolling a coarse-grained Ni-Co-Cr alloy and subsequent thermal annealing. The sample with heterogeneous microstructure exhibits simultaneously higher strength and larger uniform elongation compared with the original alloy without cold rolling. Electron backscatter diffraction, transmission electron microscopy, energy dispersive X-Ray spectroscopy, and atom probe tomography are performed to investigate the microstructural evolution of the heterogeneous structure tensile loaded to various strains, with an emphasis on the evolution of defects around the interface between nano-grains and ultrafine-grains. With a thorough comparison with the original coarse-grained sample on the deformation mechanisms, the effect of the complexity of the heterogenous microstructure on the evolution of dislocation density and deformation mechanism is illustrated, which serves to reveal the mechanisms responsible the work hardening and ductility.

*Keywords: Heterogeneous microstructure, Strength, Plasticity, Work hardening.*

# Polymer Alloying by Severe Plastic Deformation (SPD) - New Potential of Producing Materials with Exceptional Properties

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## Abstract

The need for different material properties for a given structural element from metals led to the development of alloyed metals. The basic approach so far is to alloy the selected metal with other metals, or composites by combining different materials. These procedures, however, led to the existence of hundreds of different metal alloys which made their recycling very complex, in many cases, even impossible. Sustainable metal life cycles quest the development of new processes which can reduce the number of different metals needed by using the same kind of recycling process, preferably to 100% recycling.

When a pure metal/metal-matrix composite is made with the addition of ceramic particles, it can be readily recycled. The metal properties can be tuned by particle size and volume fraction. Severe plastic deformation (SPD) processes appeared to be very promising for tailoring material properties by controlling the grain size on a large scale. It turned out, however, that the produced microstructures are not stable when the material is subjected to heat.

The present work proposes a new metal forming process in which a Metal Matrix Polymer Derived Ceramic Composite (MMPDCC) is produced with exceptional strength, ductility and thermal stability. It is applicable at much higher temperatures than that they were produced (actually, at room temperature). The process is based on interdisciplinary advances in SPD processes, powder processing, and polymer science. The obtained MMPDCC has grain sizes of the base metal in the range of 50−1000 nm with nano sized ceramic particles dispersed at the grain boundaries. This metallurgical strategy is applicable to any base metal with properties can be tuned within a large interval that opens up new avenues for developing advanced materials without complex alloy systems.

*Keywords: New Metallurgical Strategy, Polymer Alloying, Severe Plastic Deformation, Recyclable Materials*

# Technical **Oral Session _ Session 1**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 1 (N1)** **10:50 - 12:35, Nov. 20**

**Chair :** Katsuyuki MATSUNAGA (Nagoya University), Won-Seok Ko (Inha University) 203, 2F

10:50-11:20 **K-N0824** **[Keynote] Material Discovery Using Machine-Learned Potentials**
Seungwu Han (Seoul National University, Korea)

11:20-11:40 **I-N0428** **[Invited] Role of triple junctions on slip localizations in polycrystalline Ni-based superalloys**
Irene Beyerlein (University of California Santa Barbara, USA)

11:40-12:00 **I-N0427** **[Invited] Crystal growth in Supercomputer: The cutting edge of large-scale molecular dynamics simulation of metallic materials**
Yasushi SHIBUTA (The University of Tokyo, Japan)

12:00-12:20 **I-N1153** **[Invited] The effect of atomic hydrogen on the behavior of a single dislocation of <111>{112} in bcc tungsten: atomistic study**
Keonwook Kang (Yonsei University, Korea)

12:20-12:35 **O-N0670** **Molecular dynamics analysis of interaction between screw dislocation motion and hydrogen diffusion in BCC iron**
Shuhei Shinzato (Osaka University, Japan)

# Material Discovery Using Machine-Learned Potentials

**Seungwu Han**[1]

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**Abstract**

The high accuracy of the density functional theory (DFT) method allows for evaluating free energies at various conditions that are necessary for constructing the phase diagram and identifying crystal structures of unknown compounds. However, computational costs in obtaining entropic contributions and exploring huge configuratinal spaces are prohibitively expensive with DFT method. Recently, machine-learned potentials successfully demonstrated high efficiency and sufficient accuracy in free energy calculations. In this presentation, using neural-network interatomic potentials, we present recent achievements from our group along this direction. First, we develop crystal structure prediction of completely unknown compounds by employing neural network interatomic potentials as a high-fidelity surrogate model of DFT. Since the crystal structure is unknown, we construct the training set using disordered phases such as liquids and amorphous structures. We confirm that the neural network potentials can rank various metastable structures properly. By combining the neural network potential and evolutionary algorithm, we search the equilibrium structure of various test compounds. We also examine synthesizability of unknown chemical space in ternary metal oxides. Next, we present the construction of archetypal MgO-CaO eutectic phase diagram. The free energies are evaluated by the thermodynamic intergration method or semi-grand ensemble methods. The resulting phase boundaries agree very well with the known experimental data.

*Keywords: Material discovery, phase diagram, machine-learned potential, free energy.*

# Role of triple junctions on slip localizations in polycrystalline Ni-based superalloy

**Irene J. Beyerlein**[1], Jonathan Hestroffer[2], Marie-Agathe Charpagne[3], Jean-Charles Stinville[4], Matthew P. Miller[5], Tresa M. Pollock[6]

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## Abstract

Under mechanical monotonic or cyclic strain, slip can localize within individual grains, creating intense slip bands that can eventually serve as precursors for cracks. Experimental, statistical, and computational analyses have frequently correlated their locations with properties of the parent grain, including grain orientation, shape, and size, as well as subgrain features, such as proximity to triple junctions, sharp corners, and neighboring twin boundaries. Yet, to date, better understanding of the spatially and temporally resolved patterns of slip that result in the severest irreversible changes is desired. In our recent work, we studied incipient slip localization in the vicinity of hundreds of grain boundary triple junctions (TJs) in a lightly deformed nickel-base superalloy IN718 using a combination of 3D crystal plasticity finite element (CPFE) modeling, high resolution digital image correlation and 3D electron back-scatter diffraction tomography. The talk will present a large-scale CPFE model of the experimental 3D microstructure composed of high-fidelity representation of the TJ lines and the boundaries and interiors of the parent grains and use it to calculate the local micromechanical response and slip activity of all TJs at the onset of macroscopic yielding. Statistical analysis of the calculated quantities reveals that TJs develop larger stress concentration and grain-average re-orientation than the grain interiors and grain boundaries. TJs with observed slip bands generate lower grain-average re-orientation, fewer active slip systems, and more localized slip on a single system than those without. The distinctions in the reorientation and slip activity are stronger in TJs that experience more intense slip.

*Keywords: Microstructure, superalloys, rare events, micromechanics, slip.*

# Crystal growth in Supercomputer: The cutting edge of large-scale molecular dynamics simulation of metallic materials

**Yasushi Shibuta**[1]

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**Abstract**

In recent years, the spatial scale that can be handled by numerical simulations has been greatly extended due to the dramatic improvement of the computing environment. The authors have realized an all-atom analysis of the microstructure of materials on the micrometer−scale using more than 10 billion atoms by ultra-large scale molecular dynamics (MD) simulations on a supercomputer [1]. In general, the primary information obtained from MD simulations is only the coordinates and velocities of atoms. As simulations become larger in scale, post-analysis, storage, and reuse of the huge amount of data output from MD simulations are becoming a new challenge. Therefore, the authors have been investigating new analytical methods based on data science and statistical methods. In particular, we have developed new methods for utilizing MD data, such as estimating interfacial property parameters by data assimilation between MD data and the phase-field method (PFM) [2], and dimensionality reduction and restoration of MD data using a deep generative model [3]. In addition, coarse-grained MD was employed to achieve micrometer-scale crystal growth from atomistic viewpoint [4], which results in the dendrite growth directly from atomic simulations. In the talk, these recent achievements will be presented.
[1] Y. Shibuta et al., Nature Comm. 8 (2017) 10. [2] Y. Nagatsuma et al., Nanomaterials 1 (2021) 2308. [3] K. Sase, Y. Shibuta, to be submitted. [4] L. Chalamet et al. submitted.

*Keywords: Molecular dynamics simulation; Crystal growth; Machine Learning; Deep Generative Model.*

# The effect of atomic hydrogen on the behavior of a single dislocation of <111>{112} in bcc tungsten: atomistic study

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## Abstract

Tungsten (W) has been widely studied and spotlighted as a plasma-facing material (PFM) in the extreme environment of nuclear fusion due to its excellent physical properties. It is important to investigate the effect of hydrogen on the material behavior of tungsten as it was used in the hydrogen-rich fusion environment Solute hardening is a typical phenomenon and it is traditionally understood by dragging or pinning effect when hydrogen atoms act like solute atoms that impede dislocation motion. On the other hand, there were several experimental studies reporting softening associated with enhanced dislocation activity, either by easy nucleation or increased mobility, or both. In order to shed light on these controversial observations, the authors focused on the hydrogen effect on dislocation mobility in W using molecular dynamics simulations with different dislocation types, hydrogen concentrations, stress, and temperature. At high concentration of 1 at.%, H atoms are often strongly clustered around a dislocation core and produce a super-pinning effect in that both edge and screw started to move at a stress far beyond Peierls stress. This critical stress reduces with temperature increase, and thermally assisted kink or jog formation helps a dislocation escape from the H-cloud trapping. At a low concentration of 0.01-0.1 at.% or a high concentration of 1 at.% without super-pinning, hydrogen dragging barely appeared with a screw dislocation, and the intrinsic lattice resistance dominated the motion of a screw. For an edge dislocation under the same condition, an appreciable reduction in mobility was observed with the increase of H concentration at a low temperature of 300 K and this change in mobility becomes inconspicuous for higher temperatures. In conclusion, this study predicts the hardening of W at a high H concentration of 1 at.% due to dislocation trapping at the H cluster.

*Keywords: Molecular dynamics; Peierls stress; Dislocation mobility; Solute drag; Tungsten.*

# Molecular dynamics analysis of interaction between screw dislocation motion and hydrogen diffusion in BCC iron

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## Abstract

Hydrogen affects the mechanical properties of metallic materials, and these effects are known as hydrogen embrittlement. Since iron and its alloys are widely used in industry as structural materials, it is essential to understand the mechanism of hydrogen embrittlement. In iron and other body-centered cubic metals, plastic deformation is governed by the motion of screw dislocations, and it is important to understand the effect of hydrogen on the behavior of screw dislocation dislocations.

To study the dislocation behavior influenced by hydrogen and vacancy, molecular dynamics simulation is one of the effective ways to analyze the interaction between defects. However, the empirical potentials typically used in molecular dynamics are less reliable since most of them can not reproduce energy profiles of screw dislocation core and hydrogen diffusion around vacancy obtained by first-principles density functional theory (DFT) calculations. Meng et al. recently proposed the neural network interatomic potential for the iron-hydrogen system which reproduces DFT results well for the properties of screw dislocations and hydrogen-dislocation interactions.

In this study, we analyze the motion of screw dislocation with hydrogen and vacancy interactions based on molecular dynamics using the neural network potential of Meng et al. In the analysis of dislocation motion in hydrogen without initial vacancies, it was observed that dislocations move on a single slip plane in pure iron. In contrast, cross-slip occurs at various sites along the dislocation line in the case of a hydrogen environment, which promotes jog dragging and point defect nucleation.

*Keywords: Hydrogen embrittlement, BCC Iron, Molecular Dynamics, Screw Dislocation, Machine-Learning Interatomic Potential*

# Technical **Oral Session _ Session 1**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 1 (O1)** 10:50 - 12:25, Nov. 20

**Chair:** Jing Liu (Wuhan University of Science and Technology/ ShenZhen University) 401, 4F

10:50-11:20 **K-O0798** **[Keynote] Turquoise Hydrogen Production Route for Green Steel**
Youn-Bae Kang (Pohang University of Science and Technology, Korea)

11:20-11:40 **I-O0800** **[Invited] Thermodynamics of Sulfide phase in Molten Fe–Cr–Mn Alloy**
Takahiro MIKI (Tohoku University, Japan)

11:55-12:10 **O-O0032** **Study on Reuse Technology of Cold Casting Residue in the Refining**
Hao Ning (Research Institute of Technology, Shougang Group Co., Ltd., China)

12:10-12:25 **O-O0308** **New Carbon Recycling Ironmaking Process using Carbon-Iron Ore Composite**
Taichi Murakami (Tohoku University, Japan)

# Turquoise Hydrogen Production Route for Green Steel

**Youn-Bae Kang**[1], Tae-Gyu Wi[2], Young-Joon Park[3], Uendo Lee[4]

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**Abstract**

The production of "Green Steel" necessitates the reduction of $CO_2$ emissions throughout the entire steel production and processing. Although new technologies for ironmaking and steelmaking processes have been proposed, focusing on the utilization of $H_2$, the feasibility of obtaining sufficient $H_2$ with reduced $CO_2$ emissions and reasonable costs remains uncertain. The conventional Steam Methane Reforming (SMR) technology, which has been the primary method for $H_2$ production, is expected to be replaced by more competitive alternatives that emit less $CO_2$ and require lower energy input. One promising technology for $H_2$ production without $CO_2$ formation is the pyrolysis of natural gas. Among various options, the utilization of a bubble column reactor with liquid metal as a catalyst has recently garnered attention. This presentation aims to review the production routes of different variants of turquoise $H_2$, including the bubble column reactor. Specifically, it will discuss the assessment of catalytic molten metal selection, incorporating a novel experimental approach for this selection process.

*Keywords: Green steel, turquoise $H_2$, catalyst, molten metal*

# Thermodynamics of Sulfide phase in Molten Fe–Cr–Mn Alloy

**Takahiro MIKI**[1]

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**Abstract**

Phase equilibria in Fe–Cr–Mn–S quaternary system were investigated experimentally. Two liquid phases: molten metal alloy phase and molten sulfide phase were in equilibrium in this system. The equilibrium relations between molten metal alloy and sulfide phases were experimentally measured. By using metal/sulfide equilibrium method, activity of constituents in molten MnS–CrS–FeS sulfide phase were determined. By utilizing regular solution model, activity curves of constituents in sulfide phase were estimated. Thermodynamic property of solid MnS–CrS–FeS system was determined based on the combination between thermodynamic properties of liquid MnS–FeS, CrS–FeS, and MnS–CrS–FeS phase determined by the authors and reported phase diagram of MnS–FeS, CrS–FeS and MnS–CrS system. The determined parameters were verified by comparison with experimental results of equilibrium relationship between metal/sulfide in Fe–Cr–Mn–S system. By utilizing the determined parameters, phase equilibria involving sulfide phase in liquid Fe–Cr–Mn–S system was established. According to the phase equilibria information, controllability of MnS–CrS–FeS sulfide phase in typical stainless steel during solidification was evaluated.

*Keywords: Equilibrium, Activity, Phase Diagram, Thermodynamics, Inclusions*

# Study on Reuse Technology of Cold Casting Residue in the Refining

**Ning Hao[1],** Jingang Liu[2], Yanan Jia[3]

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## Abstract

The phases of cold casting residue after refining during the MCCR process included mainly $Ca_{12}Al_{14}O_{32}F_2$ and some $Ca_2SiO_4$ and $Ca_3SiO_5$, which has the characteristics of low melting temperature, fast melting speed, and strong desulfurization ability, so it was feasible to be returned to the refining process for reuse as desulfurizer and slagging agent, which not only reduced the pollution to the environment, and achieved better economic benefits. In this paper, the cold casting residue was crushed and sieved to 10-30mm, and then substitution of part of CaO was added into the steel stream during tapping. The whole industrial production process was: KR desulfurization pretreatment - BOF - LF refining - VD vacuum refining - continuous casting. The experiments results showed that the desulfurization rate during the tapping process was up to 39% and the slagging rate during LF refining process was improved, the sulfur content in the molten steel after the LF refining were all less than 0.005%, and less than 0.001% after VD refining, which fully meeting the requirements for the sulfur content of the test steel.

*Keywords: Cold casting residue, Refining, Desulfurization.*

# New Carbon Recycling Ironmaking Process using Carbon-Iron Ore Composite

**Taichi Murakami**[1], Ryota Higashi[2], Daisuke Maruoka[3], Yuji Iwami[4], Eiki Kasai[5]

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## Abstract

Carbon neutrality of the society is the worldwide issues. Especially, iron- and steel industry consumes a huge amount of fossil fuel because approximately 2 billion tons of steel produces in the world. Therefore, many studies have been developed such as hydrogen reduction and carbon recycling processes. Reduction of iron ore by hydrogen generates not carbon dioxide but water vapor. It leads to drastically decrease in carbon dioxide emission. However, the refining process of molten steel using converter is required to use carbon oxidation reaction while there is no carbon in the hydrogen reduction process. On the other hand, the previous carbon recycling process is that carbon monoxide produces from carbon dioxide which is obtained by the separation from the exhaust gas from blast furnace. The reduced iron can be produced by carbon monoxide, but it is very difficult to produce molten pig iron which is useful for the refining process. To produce molten pig iron, new carbon recycling ironmaking process was suggested. This process is consisted of carbon recycling system by carbon deposition using porous iron whisker and production of molten pig iron using recovered carbon-iron ore composite. The recovered carbon is composed of solid carbon and cementite. Using this recovered carbon, the composite reduced at lower temperature than that using conventional carbonaceous materials. By heating up to 1573 K, the molten pig iron nuggets were obtained on the surface of the composite sample.

*Keywords: Carbon neutrality, Reduction of ore, Carburization, Carbon-iron ore composite, Porous iron*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 2

November 20

14:00-15:30

# Technical **Oral Session _ Session 2**

## **Symposium A :** Advanced Steels and Properties

### Advanced Steels and Properties 2 (A2) — 14:00 - 15:25, Nov. 20

Chair : Jeongho Han (Hanyang University) — Halla Hall A, 3F

14:00-14:30 **K-A0206** **[Keynote] Recent trend on development of automotive high strength steels and their contribution toward carbon neutral society**
Naoki Yoshinaga (Nippon Steel Corporation, Japan)

14:30-14:50 **I-A0642** **[Invited] Microstructural design and abrasive wear behaviour of self-reinforcing high abrasion resistant steels with low hardness**
Xiaojun Xu (Southwest Jiaotong University, China)

14:50-15:10 **I-A0527** **[Invited] Microstructure control of cold-rolled DP steel sheet for high ductility considering Mn partitioning during intercritical annealing**
Tatsuya Nakagaito (JFE Steel Corporation, Japan)

15:10-15:25 **0-A1138** **Application of chemical heterogenous designing strategy on a novel maraging stainless steel**
Geng Liu (Central Iron & Steel Research Institute Limited, China)

# Mechanisms of dislocation multiplication and nano-twin formation in a thermally cycled Fe-17Mn alloy

**Young-Kook Lee[1]**, Jin-Young Lee[2], Jin-Sung Hong[3]

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## Abstract

Mechanisms of dislocation multiplication and nano-twin formation occurring during γ ↔ ε thermal cycling were investigated using Fe-17Mn alloy. Dislocations were introduced in γ austenite at grain boundaries and inside the grains during thermally-induced $\gamma \leftrightarrow \varepsilon$ transformations. Dislocations near grain boundaries were the dislocations, which constituted ε martensite and returned to grain boundaries during $\varepsilon \rightarrow \gamma$ reverse transformation, and forest dislocations introduced by plastic deformation during $\gamma \leftrightarrow \varepsilon$ transformations. Dislocations inside the grains formed by the impingement between two ε platelets and by the branching of a new ε platelet from a pre-existing ε platelet. In addition, nano-twins were observed in the γ grains after $\varepsilon \rightarrow \gamma$ reverse transformation. The nano-twinned γ structure resulted from stacking faults inside ε platelets because the stacking faults have a twin relationship with the prior γ. Therefore, the yield strength at the peak temperature of thermal cycling increased with the number of thermal cycling due to the increases in not only dislocation density but also nano-twins.

*Keywords: Martensitic transformation, Stacking faults, Dislocation, Transmission electron microscopy, Nano-twins*

# Microstructural design and abrasive wear behaviour of self-reinforcing high abrasion resistant steels with low hardness

**Xiaojun Xu[1],** Yijie Shen[2], Wei Xu[3], Sybrand van der Zwagg[4], Minhao Zhu[5]

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**Abstract**

Abrasion resistant steels combining high abrasion resistance, good cold formability and superior impact toughness are highly demanded by various applications subjected to abrasive environments. Current developments of high-end abrasion resistant steels are very oriented on the high hardness martensitic concept following the hypothesis that the abrasion resistance holds a monotonous relationship with macro hardness. However, various experimental observations have suggested that the high hardness of martensite doesn't guarantee a superior abrasion resistance comparing to multiple phase steels with a relative lower hardness owing to the brittle nature of martensite. Therefore, systematic experiments have been conducted to tailor microstructures of advanced steels and targets at a balanced microstructure composing of a soft phase (ferrite) and hard components (martensite), in which the soft phase can provide support and impart compatibility and the hard phase can share the load and resist the destructive action of abrasive particle. In addition to the dual-phase matrix, a considerable amount of retained austenite could further enhance the abrasion resistance owing to its significant strain hardening capability via the TRIP effect. In such a manner, the relative soft matrix offers good toughness and processibility while the self-reinforcing surface provides superior abrasion resistance. Of importance is to unravel the mechanism of stress (abrasion)-induced martensitic transformation and its effect on the reinforcement of abrasion resistance. The dynamic process of microstructural evolutions during abrasion process and the wear mechanism under different loading conditions have been discussed. A promising microstructure with high abrasion resistance and low hardness has been finally obtained.

*Keywords: Abrasion resistant steels; abrasion resistance; TRIP effect; microstructural tailoring; abrasive wear mechanism*

# Microstructure control of cold-rolled DP steel sheet for high ductility considering Mn partitioning during intercritical annealing

**Tatsuya Nakagaito[1]**, Takako Yamashita[2], Shinjiro Kaneko[3]

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## Abstract

High ductility is required in high-strength steel sheets for automobiles from the viewpoint of crashworthiness as well as press formability. In this study, the effect of microstructure on the ductility of cold-rolled DP steel sheets was investigated by focusing on the characteristics of ferrite, considering the Mn distribution caused by intercritical annealing, by a new FE-EPMA technique. Two kinds of ferrite were produced due to slow cooling after intercritical annealing, one being intercritically-annealed ferrite and the other transformed ferrite. Tensile strength was determined by the volume fraction of ferrite and did not depend on the compositional ratio of the annealed ferrite to transformed ferrite, while uniform elongation and local elongation increased with an increasing ratio of transformed ferrite. This increase in uniform elongation is attributed to the suppression of necking due to the increased work hardening rate in the high strain region during tensile deformation. The high work hardening rate of this steel can be caused by misfit strain stored at the boundary due to the discontinuous change in the Mn concentration between the annealed and transformed ferrite. The increase in local elongation is attributed to the suppression of void formation at the interface between the transformed ferrite and martensite compared to that between the annealed ferrite and martensite.

*Keywords: dual phase, intercritical annealing, ductility, strain hardening, void*

# Application of chemical heterogenous designing strategy on a novel maraging stainless steel

Jie Su[1], **Geng Liu[2]**

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## Abstract

Metastable austenite plays an important role in improving the cryogenic impact toughness of maraging steels by strain-induced martensitic transformations. However, a significant volume fraction of austenite decreases the yield strength of the material. In this study, to overcome the strength-toughness issue in maraging steels, austenite with a compositional core-shell structure and specific volume fraction are designed in Fe-Cr-Ni-Co-Mo maraging stainless steel. The core-shell compositional structure comprises retained austenite with bulk content in the core region and high Ni content reverted austenite layers in the shell region. During tensile testing, a step transformation of austenite with a continuous lattice is observed; herein, the shell regions are preserved. In contrast, the core regions transform to martensite. Close to the impact fracture, the thin austenite shell layers are retained from the martensitic transformation, which further contribute to the impact toughness. Under the combined influence of austenite and nanoprecipitates (Laves phase), the investigated alloy reaches a yield strength >1200 MPa with good cryogenic impact toughness (77 K, >90 J), thereby outperforming conventional maraging steels and several high-entropy alloys. The current study demonstrates that the chemical heterogeneity within metastable austenite may create unique mechanical properties in structural materials.

*Key words: maraging stainless steel, retained austenite, austenite reversion, chemical heterogenous, precipitation.*

# Technical **Oral Session _ Session 2**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 2 (B2)** **14:00 - 15:05, Nov. 20**

**Chair** : Wei Xu (Northeastern University), Muhammad Faizan (CSIRO Manufacturing) 301, 3F

14:00-14:20 **I-B0491** **[Invited] Benefits of in situ electro-plastic treatment for rapid reduction of porosity and brittleness in cold sprayed CP Ti and Ti-6Al-4V structures**
Muhammad Faizan (CSIRO Manufacturing, Australia)

14:20-14:35 **O-B0118** **Direct Observation of Solidification in TiAl Alloys**
Tomohiro Nishimura (Kobe Steel, Ltd., Japan)

14:35-14:50 **O-B0173** **Solidification sequence of practical TiAl-based casting alloys**
Ryoji Katsube (Kyoto University, Japan)

14:50-15:05 **O-B0040** **Study on gas-based reduction behavior of low grade vanadiferous titanomagnetite with high titanium**
Jinsheng Liu (Northeastern University, China)

# Benefits of in situ electro-plastic treatment for rapid reduction of porosity and brittleness in cold sprayed CP Ti and Ti-6Al-4V structures

Saden H. Zahiri[1], **MUHAMMAD FAIZAN-UR-RAB[2]**, Mohammed Abdul Khalik[3]

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## Abstract

Titanium (Ti) has broad range of applications in biomedical, transport, aerospace, and space due to its high corrosion resistance and high strength to weight ratio. Cold spray robotic additive technology that provides high (+10kg/hr) deposition rates has become a favourable choice to manufacture Ti components. Cold sprayed additively manufactured (CSAM) components using commercially pure (CP) titanium (Grade 2 Ti) and Ti-6Al-4V (Grade 5 Ti) powders are generally porous and brittle in nature. An energy-intensive and rather expensive heat treatment process under controlled environment is required to improve the microstructure and mechanical properties of such components. Recently a cost-effective and efficient in situ electro-plastic treatment (ISEPT) has been developed to simultaneously eliminate porosity and brittleness in CSAM CP-Ti and Ti64. In ISEPT, deformation load and electric current were applied in the same direction (in situ) to introduce electro-plastic effect for dynamic recrystallisation of the CSAM structure. Results showed that the rapid heating and cooling in ISEPT prevented oxidation of titanium and to a greater extent eliminated the need for expensive inert gas or vacuum environment. Porosity of cold-sprayed Grade 2 Ti was significantly reduced from 5% to 0.1% after double ISEPT. A similar reduction in porosity was observed for CSAM Grade 5 Ti after 6 ISEPT passes. Tensile tests confirmed the drastic change in materials mechanical properties from brittle to ductile after transformation of cold spray splat structure to dense recrystallised grains. Transformation of CSAM Ti through the ISEPT process in relation to elimination of splat boundaries will be demonstrated.

*Keywords: Cold spray additive Manufacturing, Electro-plastic, CP Titanium, Ti-6Al-4V, Recrystallization.*

# Direct Observation of Solidification in TiAl Alloys

**Tomohiro Nishimura**[1], Hitoshi Ishida[2], Hideyuki Yasuda[3]

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## Abstract

TiAl alloys have been used in a wide range of applications such as aircraft engine parts and its application are expected to expand in the future. Ti-Al binary system undergoes a complex solidification process, including the formation of a γ phase (TiAl intermetallic compound) in addition to an α phase (HCP) and a β phase (BCC) depending on Al composition. Therefore, although there are various possibilities for phase selection and microstructure formation during the solidification process, the solidification process has not been empirically clarified.

Direct observation (time-resolved and *in-situ* observation) of solidification using X-ray imaging is a powerful technique to empirically understand the solidification process of metallic materials. This technique has been applied to the observation of such as aluminium alloys and Fe-based alloys.

Figure 1 shows a transmission image of the solidification process. The material was cooled at a constant rate of 0.83 K/s from 10 seconds after the start of imaging. In this observation, the primary α phase solidified as equiaxed crystals. According to the phase diagram generated by Thermo-Calc, the primary phase is the β phase. However, as a result of the reaction between TiAl and MgO, the primary phase became the α phase. The characteristic of nucleation of the α phase at small undercooling was also revealed.

Therefore, we used single crystal MgO as the sample holding container to suppress the reaction with the reactive molten Ti as much as possible, and for the first time, we successfully observed the solidification process of TiAl alloys.

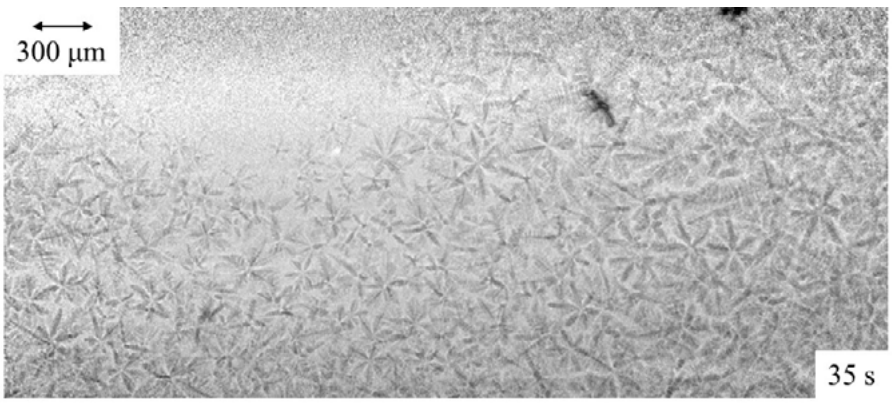



Fig.1 Transmission image of the solidification process.

# Solidification sequence of practical TiAl-based casting alloys

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## Abstract

TiAl-based alloys are a class of materials that have been intensively studied for a lightweight and high-temperature structural applications such as turbine blades for jet engines and turbine wheels for automotive engines. Since TiAl-based alloys are composed of two or more intermetallic phases, including TiAl with an $L1_0$ structure and $Ti_3Al$ with a $D0_{19}$ structure, evolution of the microstructure is rather complicated. According to the phase diagram, the multiphase microstructures are formed by a peritectic reaction, a precipitation reaction, and an order-disorder phase transformation, where the transformation rates are determined by diffusion in solids and interface kinetics. Thus, the solidification and phase transformation sequences in the practical solidification processes can deviate from the equilibrium path, and it is of interest to elucidate them. With this motivation, we have recently developed a method to observe solidification phenomena in TiAl-based alloys in the temperature range from 1173–1873 K by means of time-resolved X-ray tomography and synchronized time-resolved X-ray diffraction. In the present study, we investigated the solidification and phase transformation sequence in the second-generation TiAl-based casting alloys such as Ti-48Al-2Cr-2Nb using this procedure. As a result, we found that bcc-hcp coexisting dendrites grow from the liquid phase in the initial stage of cooling from the molten state. We also showed that the precipitation of the $L1_0$ phase from the hcp matrix coincides with the order-disorder phase transformation from the hcp structure to the $D0_{19}$ structure, which is different from the expectations based on the equilibrium phase diagram.

*Keywords: TiAl-based alloys, Solidification, Phase transformation, Time-resolved X-ray tomography, Time-resolved X-ray diffraction,*

# Study on gas-based reduction behavior of low grade vanadiferous titanomagnetite with high titanium

**Jinsheng Liu**[1,2], Zhenxing Xing[1,2], Zhuang Huan[1,2], Gongjin Cheng[1,2], Xiangxin Xue[1,2], Xueyong Ding[1]

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## Abstract

This paper proposes a procedure of $H_2$ and CO mixed gas reduction to deal with the low grade vanadiferous titanomagnetite with high titanium (LVTM) from western region of China's Liaoning province, and investigates its reduction behavior. The optimal reduction conditions were determined by analyzing of metallization rate, phase transition, and micromorphology. The results demonstrated that increasing the reduction temperature can dramatically enhance the metallization rate at first, but too high a temperature can reduce the metallization rate, the ideal temperature for gas reduction is 1323 K. The metallization rate was first characterized by a sharp increase with the extension of the reduction time, and followed by a gradual deceleration after reaching a plateau, the optimal reduction time is 90 min. The metallization rate rises with the percentage of $H_2$ content while the total amount of $H_2$ + CO gas remains stable, sharply increasing from 48.99 % when $H_2$/CO is 0 to 95.36 % at $H_2$/CO of 1.5. The titanium-bearing minerals in the LVTM, such as titanomagnetite and ilmenite, were transformed into metallic iron and titanium oxides after the reduction, and which realized the separation of metallic iron from other grains of pulsatiles such as titanite. However, most of the titanium-bearing minerals do not completely separate, but are instead interspersed in the metallic iron pores, greatly increasing the subsequent separation and recovery of iron and titanium.

***Key words:*** *LVTM, $H_2$/CO, reduction behavior, metallization rate*

# Technical **Oral Session _ Session 2**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 2 (C2)** **14:00 - 15:35, Nov. 20**

**Chair :** Da SHU(Shanghai Jiao Tong University) 201A, 2F

14:00-14:30 **K-C0709** **[Keynote] Development of Environmental Resistant Ni Base Superalloys using Artificial Intelligence Approach**
Youngsoo Yoo (Korea Institute of Materials Science, Korea)

14:30-14:50 **I-C0882** **[Invited] Effect of Ru addition on the microstructural stability and creep properties in nickel-based single crystal superalloys**
Jinguo LI (Institute of Metal Research, Chinese Academy of Sciences, China)

14:50-15:05 **O-C0861** **Composition optimization of Inconel 718 via cluster formula and experimental verification**
Yancheng Li (Dalian University Of Technology, China)

15:05-15:20 **O-C0180** **Microstructure evolution of Ni-base single crystal superalloys at high temperature and resulting viscoplastic properties: Experiments and Modelling**
Shamanth Shiva Kumar (Université Paris-Saclay, France)

15:20-15:35 **O-C0453** **High-cycle fatigue behavior of a coated third-generation single crystal superalloy at 900°C**
Dong Sun (University of Science and Technology Beijing, China)

# Development of Environmental Resistant Ni Base Superalloys using Artificial Intelligence Approach

**Youngsoo Yoo[1],** Hiwon Jeong, Seongmoon Seo, Daewon Yun, Hyungsoo Lee

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**Abstract**

High temperature environmental resistance is a crucial requirement for the structural materials for future energy plant applications. Statistical data modeling can be a powerful tool in alloy design provided reliable database is available. When there is no previous database, large numbers of experiments are needed to construct new database. Design of experiment such as Box-Behnken design can be an efficient method for the new database generation if the number of inputs is large. After considerate construction of corresponding data base, training of the data is followed to predict various properties accurately for unseen input. A number of case studies of application of artificial intelligence approach are presented including compositional optimization for high temperature environmental resistant Ni base superalloys.

*Keywords: Ni Base Superalloys, Oxidation, Neural Network, Alloy Design, Design of Experiment*

# Effect of Ru addition on the microstructural stability and creep properties in nickel-based single crystal superalloys

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## Abstract

The effect of Ru on structural stability and creep properties has been investigated in two single crystal (SX) superalloys with different Ru additions (0Ru and 2Ru in weight percent). The effect of Ru on the formation of topologically close-packed (TCP) phase is related to the location of long-term thermal exposure samples: Ru inhibits it inside the samples by "reverse partitioning" mechanism, but promotes it in the near surface regions because Ru exacerbates the oxidation. Ru can increase the creep life at 1140 ℃. Interestingly, subgrain boundaries or low angle grain boundaries (LAGBs) were observed in the γ and γ′ phases at the tertiary stage of creep, and even large angle grain boundaries (HAGBs) were observed near the fracture surface, indicating the occurrence of dynamic recrystallization (DRX). The LAGBs inside the γ and γ′ phases are formed of dislocation networks composed of single dislocations and superdislocation pairs, respectively. Ru can reduce stacking fault energy, promote the dissociation of dislocations in both γ and γ′ phases, hinder the climb and cross slip of dislocations, delay dynamic recrystallization (DRX), and thus improve the high-temperature creep resistance. In addition, Ru has a particularly significant improvement in the creep strength at 760 ℃. Because the low stacking fault energy of the Ru-containing alloy can promote dislocation dissociation and form stacking faults in both horizontal and vertical channels, thereby inhibiting the nucleation of a<112> dislocation ribbons and reducing the primary creep strain.

*Keywords: Nickel-base single crystal superalloys; creep; ruthenium (Ru); topologically close packed (TCP) phase; subgrain boundaries.*

# Composition optimization of Inconel 718 via cluster formula and experimental verification

**Yancheng Li** [1], Qing Wang [2], Ying Li [3], Chuang Dong [4]

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## Abstract

Superalloys feature multi-elements and complex elemental ranges, which makes the proper compositio selection difficult. In fact, more strict composition standards generally apply in practical productions The objective of this paper is to understand and eventually to renew the composition standard vi example of the most common grade Inconel 718. We have recently shown that the alloy chemistr originates from a nearest-neighbor cluster [center-shell] plus a few next-neighbor glue atoms, o expressed in cluster formula [center-shell](glue atoms). By grouping the elements into $\overline{Ni}$ = (Ni, Co Cu, Fe), $\overline{Cr}$ = (Cr, Mn, Si, Mo), and $\overline{Nb}$ = (Nb, Al, Ti), it is found that the reported alloys fall withi a narrow composition zone $\overline{Ni}_{11.0\sim13.0}$-$\overline{Cr}_{3.5\sim4.5}$-$\overline{Nb}_1$ confined by cluster formulas of 16 and 18 atoms This composition zone is also expressed in terms of 288-atom supercluster formulas, $\overline{Ni}_{198\sim208}$-$\overline{Cr}_{63\sim72}$ $\overline{Nb}_{16\sim18}$, which lead to coordinated elemental variations in wt.%: 69.0 ≤ Ni + Co + Cu + Fe ≤ 72.7; 19.8 ≤ Cr + Mn + 1.7 Si + 0.6 Mo ≤ 22.8; 8.7 ≤ Nb + 3.2 Al + 1.9 Ti ≤ 9.8. Within this composition zone $\overline{Ni}_{206}$-$\overline{Cr}_{65.5}$-$\overline{Nb}_{16.5}$ is further pinpointed and validated by our own experiments to possess the optima match of strength and plasticity both at room and at 923K.

*Keywords: Inconel 718 superalloy; cluster-plus-glue-atom model; cluster formula; composition standard*

# Microstructure evolution of Ni-base single crystal superalloys at high temperature and resulting viscoplastic properties: Experiments and Modelling

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**Abstract**

The use of nickel base single crystals superalloys for turbine blade applications allows higher thermal efficiency and greater thrust/mechanical power. But these high temperature cycles degrade the blades and cause catastrophic failure. Hence the engine is subjected to a series of validation tests dictated by FAA/EASA to determine its airworthiness especially for the case of One Engine Inoperable situations. Decades of research on this class of material currently allow us to use constitutive models but the major portion of anisothermal response of the material remains to be explored.

The present study focuses on improving an existing model (coupling with viscoplasticity, damage and rafting phenomenon) by adding anisothermal effects (in thermodynamics framework) and performing additional mechanical tests at high temperatures. This includes a series of relaxation tests to study the initial microstructure influence on the stress relaxation and damage evolution for iso and anisothermal creep tests. An emphasis is made on the evolution of microstructure during load free condition for pre-crept samples.

*Keywords: single crystals, high temperature creep, relaxation, damage, rafting.*

# High-cycle fatigue behavior of a coated third-generation single crystal superalloy at 900℃

**Dong Sun[1],** Siliang He[1], Weiwei Zheng[1], Longfei Li[1], Song Lu[1], Jonathan Cormier[2], Qiang Feng[1]

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**Abstract**

High-cycle fatigue (HCF) is one of the primary failure modes of turbine blades in aero-engines. Therefore, comprehending the effect of coating on the HCF property of single crystal (SX) superalloys is vital for the safe service of turbine blades. This study investigated the effect of PtAl coating on HCF properties and crack initiation process of Ni-based SX superalloy DD90 with thin-walled geometry at 900 ℃ and varying stress amplitudes. The results indicated that both coating and stress amplitude significantly affected fatigue properties and crack initiation process of DD90 alloy. Fatigue crack initiation sites of both uncoated and coated alloys transformed from internal casting pores to surface cracks with the decreased stress amplitude. However, the coating significantly increased the stress amplitude required for the transformation of the fatigue crack initiation site. Meanwhile, PtAl coating caused damage to the HCF property of under low-stress amplitude, which got progressively severe with decreasing stress amplitude. In a word, the brittle cracking of the coating facilitated the rapid nucleation of surface cracks, which promoted the transformation of the fatigue crack initiation site from casting pore to surface crack under higher stress amplitude, due to the introduction of PtAl coating. On the other hand, grain boundaries in interdiffusion zone (IDZ) and oxidation at the crack tip accelerated the growth of surface crack under low-stress amplitude, resulting in a lower fatigue life of the coated alloy. This work will be helpful in accurately predicting the HCF life of the coated SX superalloys.

*Keywords: Ni-based single crystal superalloy, PtAl coating, high-cycle fatigue, crack initiation, surface microcrack.*

# Technical **Oral Session _ Session 2**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 2 (D2)** **14:00 - 15:35, Nov. 20**

**Chair :** Hyunjoo Choi (Kookmin University), Bernard Rolfe (Deakin University) Samda Hall A, 3F

14:00-14:20 **I-D1050** **[Invited] Effect of Cu on precipitation of α-Al(Mn,Cr)Si dispersoids in Al-Mg-Si-Mn-Cr alloys**
Nagaumi Hiromi (Soochow University, China)

14:20-14:35 **O-D0524** **Microstructure and tensile properties of Al-Mg- Si alloy fabricated by horizontal and vertical twin-roll casting**
Jo YongHee (Korea Institute of Materials Science, Korea)

14:35-14:50 **O-D0259** **Improvement of formability of silicon-containing recycled wrought aluminum alloy by hot stamping after rapid heating**
Ryohei Kawana (Yokohama National University, Japan)

14:50-15:05 **O-D0192** **Optimization of heat treatment process to improve mechanical properties and thermal stability of extruded Al-Mg-Si Alloy**
Jisu Kim (Korea Institute of Materials Science, Korea)

15:05-15:20 **O-D0394** **In-situ nanostructure analysis of 7000 series aluminum alloys aging at low temperature**
Tomomi Suzuki (Hokkaido University, Japan)

15:20-15:35 **O-D0532** **Enhanced strength and conductivity of Al-Mg-Si alloys with optimized Mg/Si ratio and artificial aging treatment**
Qipeng Dong (Soochow University, China)

# Effect of Cu on precipitation of α-Al(Mn,Cr)Si dispersoids in Al-Mg-Si-Mn-Cr alloys

**Hiromi Nagaumi[1],** Fangzhen Liu[1], Qipeng Dong[1], Jian Qin[2]

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## Abstract

Nanoscale α-dispersoids in aluminum alloys play a crucial role in enhancing the mechanical properties of the alloys. In this study, the effect of adding 0.6 wt% copper (Cu) on the precipitation behavior of α-dispersoids in Al-Mg-Si-Mn-Cr alloys during homogenization heat treatment at 500/560 °C was investigated. After the homogenization process, both alloys exhibited a significant number of α-Al(MnCr)Si dispersoids with various morphologies, such as cubic, rod-like, and disc-like shapes. However, the alloy with the addition of Cu exhibited a higher density of α-dispersoids, and these dispersoids were relatively smaller in size compared to the alloy without Cu. Importantly, the transmission electron microscopy (TEM) results revealed that the Cu addition promoted the precipitation of cubic dispersoids with a quasicrystalline structure. This suggests that Cu has a favorable influence on the formation of these specific dispersoids. Consequently, the alloy with 0.6 wt% Cu addition exhibited a remarkable increase in yield strength of 14 MPa (equivalent to a 42.4% improvement) at an elevated temperature of 300 °C. This study provides new insights by demonstrating that, in addition to precipitation strengthening, the addition of Cu in an Al-Mg-Si-Mn-Cr alloy also contributes to the precipitation of α-dispersoids. The enhanced precipitation of α-dispersoids, particularly the cubic dispersoids with a quasicrystalline structure, results in improved mechanical properties.

*Keywords: Cu alloying; α-Al(Mn,Cr)Si dispersoids; quasicrystalline structure; simple cubic structure.*

# Microstructure and tensile properties of Al-Mg- Si alloy fabricated by horizontal and vertical twin-roll casting

**Yong Hee Jo[1],** Jae Wung Bae[2], Jisung Yoo[3], Seok Gyu Lee[4], Hyoung-Wook Kim[5]

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**Abstract**

In this work, Al-Mg-Si alloys with different casting rates were fabricated by horizontal and vertical twin-roll casting (HTRC and VTRC). A comparative analysis of the microstructure evolution and mechanical properties between the two alloys was performed. The central segregation of the H-alloy is the channel segregation, but that of the V-alloy is the segregation band. The texture components of the H-alloy represent rolling and shear structures that represent continuous casting with hot rolling processes during the HTRC, whereas the V-alloy represents random texture that implies no hot rolling during VTRC. The plastic deformation already exists inside both the center and surface regions in the HTRC. However, the overall plastic deformation is lower in the VTRC. In both the as-cast and thermomechanically processed condition, the H-alloy shows a lower tensile strength than the V-alloy. This work aims to provide a broad understanding of TRC strips through comparative analysis of microstructural changes and tensile properties through the horizontal and vertical twin-roll casting.

*Keywords: Al-Mg-Si alloy; Twin roll casting; Casting speed; Microstructure evolution; Tensile properties.*

# Improvement of formability of silicon-containing recycled wrought aluminium alloy by hot stamping after rapid heating

**Ryohei Kawana[1]**, Shoichi Hirosawa[2], Mitsuhiro Ootaki[2], Tomoyoshi Maeno[2], Yasushi Suzuki [3] and Yuuji Yabuki [3]

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## Abstract

At present, casting and wrought aluminium alloys collected from scrapped vehicles are melted together, and thus the produced recycled aluminium ingots inevitably contain higher Si contents together with various types and amounts of impurity elements. In progress of electrification of automobiles, however, less future demand of cast and die-cast products with larger allowable concentrations of impurity elements gradually forces to utilize the ingots as wrought materials although their formability is generally inferior. In this study, therefore, the formability of Al-Si alloy sheets was aimed to be improved by hot stamping after rapid heating, and the optimum process parameters correlating amounts of Si and impurity elements with heating temperatures were also proposed.

Al-3%Si, Al-7%Si and Al-12%Si binary alloys were casted, homogenized and cold-rolled at a reduction ratio of 80%, and their mechanical properties were evaluated by a tensile test, together with those of a commercial A4032-T6 (containing 12%Si, 1%Mg, 1%Cu and 0.9%Ni) alloy sheet. Microstructural observation was conducted using optical microscope and scanning electron microscope.

Irrespective of Si contents, ultimate tensile strength of 200-210 MPa were obtained in the three cold-rolled specimens, but the elongation to fracture were all below 10%. However, such inferior ductility, in other words inferior formability, could be improved by hot stamping after rapid heating to 250˚C for Al-12%Si and A4032-T6 for V bending with a radius of 9mm. Similar improvement was accomplished for V bending with a radius of 2mm when rapid heating to 250, 300 and 350˚C is designed for Al-7%Si, Al-12%Si and A4032-T6, respectively.

*Keywords: recycled aluminium alloy, Al-Si, rolling, formability, hot stamping*

# Optimization of heat treatment process to improve mechanical properties and thermal stability of extruded Al-Mg-Si Alloy

**Jisu Kim[1],** Su-Hyeon Kim[2], Jeki Jung[3]
Hyun-Seok Cheon, Cha-Yong Lim, Yoon Suk Choi

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**Abstract**

Heat-treatable Al-Mg-Si alloys can have high strengths by precipitation hardening. These alloys have been used in the application of automobiles as structural parts due to their excellent formability and processability. However, the mechanical properties of heat-treatable Al alloys can deteriorate when they are exposed to elevated temperatures for a long time. In this study, we aimed to optimize heat treatment processes to enhance both the strengths and the thermal stability of the extruded Al-Mg-Si alloy by controlling the size and number density of precipitates. The extruded tube of the alloy was solution treated with various conditions changing the solution treatment temperature and air cooling time before water quenching. The solution treated samples were artificially aged, and further heat treated at 150 ℃ for 1000hrs to evaluate the thermal stability of the mechanical properties. Hardness measurement and tensile tests were performed for each sample. Higher temperature solution treatment and shorter air cooling time resulted in higher strengths and enhanced thermal stability of the alloy. Transmission electron microscopy (TEM) observation and Differential scanning calorimetric (DSC) analysis were also carried out to understand the influence of the size and distribution of β″ precipitates in each heat treatment process on the strengths of the alloy.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: Al-Mg-Si alloys, heat treatment, thermal stability, negative natural aging effect, mechanical property*

# In-situ nanostructure analysis of 7000 series aluminum alloys aging at low temperature

**Tomomi Suzuki**[1], Masato Ohnuma[2], Mami Mihara-Narita[3]

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**Abstract**

Since formation of the GP zone occurs at room temperature in Al-Zn-Mg alloys and Al-Zn-Mg-Cu alloys, preservation of the samples in the freezer or liquid nitrogen is often adopted for keeping quenched state. However, little is known about the microstructure development at the lower than room temperature. Therefore, in this study, four different aging temperatures from -10°C to room temperature (about 22 °C) are selected for in-situ Small Angle X-ray Scattering (SAXS) measurements after solid solution treatment to clarify the aging behavior at lower temperatures.

Al-Zn-Mg alloy and Al-Zn-Mg-Cu alloy were used as samples. After solid solution treatment at 450°C for 1 hour, the samples were water quenched (WQ) and aged at four different temperatures (room temperature, 10°C, 0°C, and -10°C) for the maximum about 60 hours.

It was confirmed that the precipitation rate decreased as the aging temperature was lowered. Aging Al-Zn-Mg alloy at -10°C, formation of GP zone did not progress for the first 3 hours. However, GP zone started and the volume fraction increased after that. Using the Johnson-Mehl-Avrami equation to determine the reaction rate constant, and utilizing the Arrhenius plot, it was calculated that the volume of precipitates at -60°C would be 10% of the room temperature. On the other hand, GP zone did not form at -10°C for 60h in Al-Zn-Mg-Cu alloy, while GP zone formed by aging at 0°C for longer than 20h.

*Keywords: in-situ Small angle X-ray scattering, low temperature*

# Enhanced strength and conductivity of Al-Mg-Si alloys with optimized Mg/Si ratio and artificial aging treatment

**Qipeng Dong[1]**, Yi Zhang[2], Hiromi Nagaumi[3]

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## Abstract

Al-Mg-Si alloys are widely used for heat-dissipation and electricity transmission due to their high strength, relatively high conductivity and low cost. Owing to the ever-increasing demands in lightweight, developing an alloy that simultaneously possesses high strength and high conductivity has recently received great attention. However, in response to the mutually exclusive characteristic between strength and conductivity, a synchronous improvement in strength and conductivity is challenging. In this study, the influence of various Mg/Si ratios and aging temperatures on the strength and conductivity was investigated. Precipitation kinetics of the alloys was comparatively analysed based on the differential scanning calorimetry thermograms. The microstructural characteristics of the alloys with different Mg/Si ratios and aging conditions were investigated using transmission electron microscopy. On this basis, the contribution of each strengthening factor on hardness and electrical resistance was elaborately discussed, and the underlying mechanism of varying Mg/Si ratio and aging conditions on the strength and conductivity of Al-Mg-Si alloys was elucidated. The results show that the excess Si improves the mechanical properties of the alloy but leads to the decrease of the electrical conductivity, while the excess Mg is detrimental to both the mechanical and electrical conductivity. A Mg/Si ratio (mass ratio) of approximately 1.0 allows sufficient precipitation of MgSi phases during high-temperature aging process with less excessive Mg and Si solutes in matrix, which ensures the high strength while bringing a synergistic increase in electrical conductivity.

*Keywords: Al-Mg-Si alloys; Mg/Si ratio; Ageing precipitation; Strength; Thermal conductivity.*

# Technical **Oral Session _ Session 2**

## **Symposium E :** Additive Manufacturing

### Additive Manufacturing 2 (E2) 14:00 - 15:35, Nov. 20

Chair : Kee-Ahn Lee (Inha University), Shanqing Xu (Swinburne University of Technology) Halla Hall B, 3F

14:00-14:30 **K-E0456** **[Keynote] Additive manufacturing of titanium alloys with exceptionally uniform mechanical properties**
Ming-Xing Zhang (University of Queensland, Australia)

14:30-14:50 **I-E0768** **[Invited] Optimizing Mechanical Properties of Additively Manufactured Aluminum Alloy through Controlled Microstructural Heterogeneity**
Kyung Tae Kim (Korea Institute of Materials Science, Korea)

14:50-15:05 **O-E0101** **Heterostructured Ti alloys with improved mechanical properties fabricated by direct laser deposition**
Yufan Zhao (Northwestern Polytechnical University, China)

15:05-15:20 **O-E1036** **Flexural behaviour of additively manufactured functionally graded SS 316L lattice beams**
Chamini Rodrigo (Swinburne University of Technology, Australia)

15:20-15:35 **O-E1182** **Recent developments in additive manufacturing of metallic glasses and their composites**
Łukasz Żrodowski (Warsaw University of Technology, Poland)

# Additive manufacturing of titanium alloys with exceptionally uniform mechanical properties

Jingqi Zhang[1], Yingang Liu[1,] **Mingxing Zhang[1],**

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**Abstract**

Additive manufacturing (AM), which creates metallic parts by successive addition of material, is shaping the future of manufacturing. However, owing to the layer-wise build fashion of AM, metallic alloys produced by AM often develop spatially dependent phases through solid-state phase transformations under the intrinsic thermal cycling. This leads to heterogeneous phase distribution, and inhomogeneous mechanical properties, presenting substantial risks to applications involving multiaxial stress states. Although post-AM heat treatment is often performed to homogenize the microstructure, it unfortunately lengthens the production cycle and, more importantly, cannot completely eliminate the mechanical inhomogeneities due to the site-specific thermal history in the as-fabricated part. Here, based on titanium − 6% aluminium − 4% vanadium (Ti−6Al−4V, in weight per cent) − the workhorse in the titanium industry − which typically exhibits spatial variation of phases along the building direction while being additively manufactured, we demonstrate a self-stabilization strategy in which we introduce commercially pure titanium (CP−Ti) powders as the main additive and iron oxide ($Fe_2O_3$) nanoparticles as the trace additive to Ti−6Al−4V feedstock powder via a surface engineering approach. Decreasing V content by increasing CP-Ti addition whilst introducing Fe through $Fe_2O_3$ in the alloy encourages in-situ decomposition of the metastable, brittle phase − which is usually distributed on the top surface of the AM fabricated part − into stable phases similar to those in the lower region, yet without the need of additional heat treatment. Our alloys with uniform self-stabilized constituent phases not only achieve uniform tensile properties, but also stand out among the conventionally and additively manufactured Ti−6Al−4V with outstanding combinations of strength and ductility. This work provides a pathway for eliminating the mechanical inhomogeneity associated with thermal cycling that is inherent to the AM process and should help to guide the design and tailoring of new alloys specifically for AM with uniform mechanical properties.

*Keywords: Additive manufacturing, titanium alloy, pure titanium, property homogeneity.*

# Optimizing Mechanical Properties of Additively Manufactured Aluminum Alloy through Controlled Microstructural Heterogeneity

**Kyung Tae Kim[1],** Yeong Seong Eom[1], Jeong Min Park[1], Jungho Choe[1,2], Hyeong Seop Kim[2,3]

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## Abstract

The Laser Powder Bed Fusion (LPBF) method of additive manufacturing has demonstrated tremendous potential in numerous industries including aerospace, automotive, military and shipbuilding, owing to its capacity for the direct production of intricate and lightweight parts. This technique has enabled significant advancements in the production of complex geometries and the creation of parts with improved mechanical properties, which were previously unattainable through rapid melting and solidifying process. Aluminum alloys are considered as key structural materials for this LPBF process due to their high specific strength and extensive range of applications. With commercially available aluminium alloys systems such as AlSi10Mg used in the LPBF process, recently, there has been a growing interest in developing Al-Zn-Mg-Cu based alloys with the aim of addressing their high sensitivity to solidification cracks. In this presentation, we will discuss two recent research studies conducted at KIMS concerning the AlSi10Mg and Al-Zn-Mg-Cu alloy systems. For AlSi10Mg, we will explore the optimization of mechanical properties by controlling the cell-boundary microstructure. Additionally, we will describe an approach to eliminate solidification cracks in the Al-Zn-Mg-Cu systems, which involves engineering dual microstructures consisting of columnar and equiaxed grains. A simplified numerical cracking model will also be briefly presented, taking into account LPBF processing parameters of Al-Zn-Mg alloy powders. Furthermore, changes in the mechanical properties and microstructural heterogeneity of both aluminium alloys would be dealt with a focus on post-heat-treatment, based on empirical data obtained at KIMS.

*Keywords: LPBF, Aluminum alloys, Microstructural heterogeneity, Mechanical Properties.*

# Heterostructured Ti alloys with improved mechanical properties fabricated by direct laser deposition

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## Abstract

For most metal structural materials, including titanium alloys, there is often an intrinsic inversion relationship between strength and plasticity, making it challenging to improve synergistically. The emerging concept of heterostructured materials is expected to solve the problem. In this study, by manipulating the composition of TC4 titanium alloy, the TC4/TC4+2.5Ni layered heterostructures were prepared using direct laser deposition additive manufacturing. The results show that the as-built microstructure of TC4/TC4+2.5Ni layered heterostructure comprises alternating columnar and near equiaxed grain layers. When subjected to lateral loading, the change in component layer thickness affects the enhancement effect of strength-plasticity optimization. When the component thickness is too large, the synergistic optimization effect of strength and plasticity is weak due to the small number of layer interfaces that hinder crack deflection. When the component thickness is too small, it tends to homogenize and is not conducive to the uneven deformation of the heterostructure and also exhibits a weak synergistic optimization effect. The appropriate component thickness (3-4 deposited layers) has evident heterogeneity in structure and composition, as well as a large number of layer interfaces. It exhibits excellent synergistic optimization effect of strength and plasticity under HDI stress, crack deflection obstruction by layer interface, and alternating distribution of soft and hard zones to suppress strain localization. This study provides a factual basis and essential theoretical support for designing heterostructured titanium alloy by direct laser deposition and optimizing strength and plasticity synergistically.

*Keywords: Additive manufacturing, Direct laser deposition, TC4/TC4+2.5Ni layered heterostructures, Strength and plasticity, Microstructure.*

# Flexural behaviour of additively manufactured functionally graded SS 316L lattice beams

**Chamini Rodrigo[1],** Shanqing Xu[1], Yvonne Durandet[1], Darren Fraser[2], and Dong Ruan[1]
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## Abstract

The emergence of novel additive manufacturing technologies facilitates the design and fabrication of meso-scale structures with complex geometries. In this study, SS 316L lattice beams with functionally graded (FG) body-centred cubic (BCC) lattice structures were fabricated using electron beam melting (EBM, Arcam A1) and tested under quasi-static bending loads. Uni-directional density grading and bi-directional density grading strategies were used in the design of FG beams by varying the density of unit cells in four layers. Uniform lattice beam consisting of unit cells with constant density was also studied for comparison. The flexural behaviour of the lattice beams was evaluated by three-point bending tests and compared with finite element models. The experimental results revealed that the flexural stiffness and strength of bi-directional lattice beams were higher than those of both uniform and uni-directional counterparts. The strength of uni-directional lattice beams is observed to be relatively low, primarily due to the easier collapse of thinner lattice layers on the impact side under the force of the indenter. The effects of the density gradient and the loading velocity on the performance of bi-directional lattice beams were further evaluated using finite element models, developed, and validated using the experimental results. Through a parametric study it has been determined that the flexural stress and the specific energy absorption capacity of bi-directional lattice beams were influenced by both loading velocity and the severity of layer density gradient.

*Keywords: additive manufacturing, functionally graded metal lattice, three-point bending, flexural behaviour, energy absorption capacity*

# Recent developments in additive manufacturing of metallic glasses and their composites

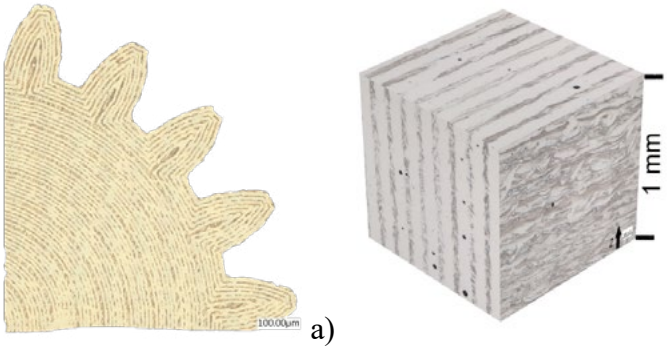
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## Abstract

Although metallic glasses (MG) have extraordinary mechanical and chemical properties, their industrial use still needs to be improved due to the low number of glass-forming alloys with high glass-forming ability (GFA), toughness, and processability.
However, the dynamic growth of laser-based Additive Manufacturing (AM) can provide a cost-effective way of producing MGs in bulk form regardless of their GFA. Although the process optimization compromises both porosity and crystallinity reduction, the non-equilibrium nature of MGs can be maintained in bulk material through high heating and cooling rates.
This trade-off has been overcome by a new AM scanning strategy and post-processing methods, which achieved high amorphous phase content with good density by finetuning double laser exposure in a key-hole mode and separating scanning lines. With selective devitrification in the heat-affected zone, fiber-like glassy-crystalline composites have been formed with full control over the microstructure.
To eliminate residual porosity without visible crystallization, hot isostatic pressing (HIP) was performed on amorphous and composite samples. This method has been successfully applied to process Zr-, Fe-, and Mg-based MGs with high and low GFA via AM. Comprehensive guidelines for MGs and their composite formation via AM are provided, including procedures for quick process optimization.




a) b)

AM processed Zr-based composite gear after HIP (a) and 4D structure of MG composite.

*Keywords: additive manufacturing, bulk metallic glasses, powder bed fusion, 4D composites, amorphous*

# Technical **Oral Session _ Session 2**

## **Symposium F :** Thin Films and Surface Engineering

### Thin Films and Surface Engineering 2 — 14:00 - 15:10, Nov. 20

Chair : Sanghan Lee (Gwangju Institute of Science and Technology), Thierry Grosdidier (Université de Lorraine) — 202A, 2F

14:00-14:20 **I-F1093** **[Invited] Advancing Ferroelectric Properties in Hafnia-Based Ferroelectrics through Interface Engineering**
Min Hyuk Park (Seoul National University, Korea)

14:20-14:40 **I-F0250** **[Invited] Advancements in Tunneling Magneto-Dielectric Effect through Additive Elements**
Cheng WANG (Tohoku University, Japan)

14:40-14:55 **O-F0285** **Hydrogen in Electrolessly Deposited Copper Films**
Shinji Yae (University of Hyogo, Japan)

14:55-15:10 **O-F0628** **Origin of Grain Refinement in Tribology**
Wenzhen Xia (Anhui University of Technology, China)

# Advancing Ferroelectric Properties in Hafnia-Based Ferroelectrics through Interface Engineering

**Min Hyuk Park**

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**Abstract**

Ferroelectric materials with a fluorite crystal structure, such as $HfO_2$ and $ZrO_2$, have captured significant attention since their discovery in 2011.[1-3] These novel materials hold promise for overcoming challenges encountered by traditional ferroelectrics, like limited scalability and compatibility issues with complementary-metal-oxide-semiconductor technology. However, the exploration of practical nanoscale ferroelectrics, particularly in the form of nanoscale solid-state devices, has underscored the critical role played by interfacial engineering.
This study investigates the impact of interfacial layers and defects on the ferroelectric properties of $Hf_{0.5}Zr_{0.5}O_2$ thin films, with a focus on both metal/ferroelectric and semiconductor/ferroelectric interfaces.[4-6] Experimental findings reveal that managing the concentration of non-ideal defects arising from interfacial redox reactions significantly influences the performance of ferroelectric devices. For example, in the metal/ferroelectric/semiconductor gate stack of ferroelectric field-effect transistors, the formation of interfacial layers with high defect concentrations emerges as a primary factor limiting endurance. Similarly, in metal/ferroelectric/metal capacitors, the presence of oxygen vacancies at interfacial regions, stemming from the oxygen scavenging effect of electrode materials, compromises optimized ferroelectric properties in their pristine state, resulting in the 'wake-up effect'.
The outcomes of this investigation emphasize the vital role of interfacial engineering in enhancing the ferroelectric behavior of $Hf_{0.5}Zr_{0.5}O_2$ thin films. By addressing the challenges posed by interfacial layers and defects, this research contributes to the advancement of fluorite-structured ferroelectrics and their potential integration into diverse nanoscale device applications."

[1] T. S. Boescke et al. Appl. Phys. Lett. 99, 102903 (2011).
[2] M. H. Park et al. Adv. Mater. 27, 1811 (2015).
[3] U. Schroeder and M. H. Park et al. Nat. Rev. Mater. 7, 653 (2022).
[4] K. Yang et al. Mater. Sci. Semicond. 164, 107565 (2023).
[5] S. H. Kim et al. Chem. Commun. 57, 23452 (2021).
[6] K. Yang and S. H. Kim et al. Chem. Mater. 35, 2219 (2023).

*Keywords: Ferroelectrics, Semiconductor, Thin Film, Atomic Layer Deposition, Interfaces*

# Advancements in Tunneling Magneto-Dielectric Effect through Additive Elements

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## Abstract

On this eve of the mid-21st century, as the global momentum for Artificial Intelligence and Sustainable Development Goals continues to grow, the magnetoelectric effect is widely studied and used as various advanced devices, including magnetoelectric random access memory, magnetoelectric energy converter, etc. Magnetoelectric materials mainly include single-phase multiferroics with coupled magnetic and electric orders, and composites consisting of magnetostrictive and piezoelectric materials. However, there remains a challenge with the requirement of extremely low temperatures and strong magnetic fields.

Recently, our group discovered a novel magnetoelectric effect, named Tunneling Magneto-Dielectric (TMD) effect, at room temperature using nanogranular film with magnetic nanogranules embedded in an insulating matrix. [Nature Communications 5,4417(2014).] Based on an entirely different mechanism, the permittivity variation originates from a spin-dependent electrical polarization due to tunneling effect. Similar tunnel magnetoresistance (TMR) effect, where the resistivity changes, has been extensively researched and applied in magnetic recording and sensing. However, TMD study is in its infancy. It is urgent to improve the performance of TMD effect with larger maximum TMD response ($TMD\%_{MAX}$) and higher TMD frequency ($f_{TMD}$) than conventional results.

In this presentation, we will review the significant advancements achieved through the additive effects of various elements to the magnetic nanogranules. Some effects act on the shape and the size of nanogranules, and has greatly improved $f_{TMD}$ from around-MHz to close-to-GHz. Others increase the spin polarization of nanogranules, and has significantly improved $TMD\%_{MAX}$ from around-5% to over-10%. These advancements have sounded a clarion call for the development of the first-generation TMD devices.

*Keywords: Magnetoelectric effect, nanocomposites, spin polarized transport, tunneling magneto-dielectric effect, additive effect.*

# Hydrogen in Electrolessly Deposited Copper Films

**Shinji Yae[1],** Kazuma Hayashi[2], Kosuke Tohda[3], Naoki Fukumuro[4]

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**Abstract**

Electroless deposition of copper is an important process in manufacturing printed circuit boards. In this process, hydrogen is generated concurrently with the deposition of copper atoms by the oxidation of reducing agent (formaldehyde). While most of them are released as molecular hydrogen bubbles, some of them are co-deposited in copper films. Hydrogen co-deposition has been recognized as cause of residual stress generation, ductility loss, and void formation in the films. However, the detailed mechanism of such hydrogen-induced phenomenon has not been clarified. We previously reported that the room-temperature grain growth observed in electrodeposited copper films is caused by hydrogen-induced superabundant vacancy-hydrogen clusters[1,2]. In this study, the atomistic state (interstitial, vacncy-hydrogen clusters, and in nanovoids) and amount of hydrogen in the electrolessly deposited copper films have been analyzed by thermal desorption spectroscopy (TDS)[3].

1) N. Fukumuro, T. Adachi, S. Yae, H. Matsuda, and Y. Fukai, *Trans. Inst. Met. Finish.*, **89**, 198 (2011). DOI: 10.1179/174591911X13082997023873

2) N. Fukumuro, H. Yoshida, T. Yamazaki, Y. Fukai, and S. Yae, *J. Japan Inst. Met. Mater.*, **80**, 736 (2016). DOI: 10.2320/jinstmet.JD201608

3) N. Fukumuro, K. Tohda, and S. Yae, *J. Electrochem. Soc.*, **169**, 122505 (2022). DOI: 10.1149/1945-7111/acaa63

*Keywords: Electroless Copper Films, Hydrogen Co-Deposition, Thermal Desorption Spectroscopy, Vacncy-Hydrogen Clusters, Nanovoids.*

# Origin of Grain Refinement in Tribology

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**Abstract**

The near-surface region of tribo-elements' microstructural modification has a substantial impact on how long a tribo-system would endure. A fundamental understanding of microstructure evolution under local tribological exposure is necessary to design and customize future surfaces of tribo-elements. Horizontal dislocation walls have been seen during the early stages of the macro-tribological process in metals, which eventually grow into the grain-refined tribolayer, but their underlying mechanisms are yet unclear. In this study, we created a brand-new micro-tribological test to more easily assess the stress condition and directly check the contact zone. Our basic tribological preliminary tests show the microscale mechanism of the creation of a horizontal dislocation wall during the tribological process and identify grain orientation and twin boundary effects in a dry environment. Our understanding of macroscale tribology can be improved by this fundamental microscale research, which can also make recommendations for reducing replacement costs, noise levels, and energy consumption in dry environments.

*Keywords: Nanotribology; Dislocation wall; Metal; Microstructure evolution*

# Technical **Oral Session _ Session 2**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 2 (G2)** **14:00 - 15:25, Nov. 20**

Chair : Ji-woon Lee (Kongju National University), Young-Bum Chun (Korea Atomic Energy Research Institute) 303A, 3F

14:00-14:30 **K-G0756** **[Keynote] Development of Metal-Coated Zircaloy for Accident-Tolerant Fuels**
Hiroaki ABE (The University of Tokyo, Japan)

14:30-14:50 **I-G1014** **[Invited] The development of interatomic potentials and simulations of primary radiation damage for vanadium alloy**
Huiqiu Deng (Hunan University, China)

14:50-15:10 **I-G0881** **[Invited] Distinct irradiation resistance mechanisms of high entropy alloys**
Chenyang Lu (Xi'an Jiaotong University, China)

15:10-15:25 **O-G0551** **Study on Phase Stability and Mechanical Properties in Mn-Ni-Si Model Alloys under Thermal Aging and Irradiation**
XINRUN CHEN (Nagaoka University of Technology, Japan)

# Development of Metal-Coated Zircaloy for Accident-Tolerant Fuels

Hiroaki ABE [1]

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**Abstract**

In the Fukushima Daiichi nuclear plant accident, the core meltdown was caused due to the thermal feedback of the oxidation reaction of the fuel cladding tubes. In recent years, therefore, the development of accident-tolerant fuels (ATF) became one of the interests. In this project, we focus on the development of metal-coated Zr alloys, which are considered most feasible in the near term. Despite the rich knowledge in Zircaloy, the knowledge is limited in the coating metal (Cr) and its interface with base materials. Our research is therefore focused to acquire knowledge for fuel cladding development, such as material design, manufacturing, mechanical strength, corrosion property, and irradiation behavior. The purpose of this presentation is to review our recent research activities.

[Material design and mechanical strength] Diffusion bonding and/or pulsed-laser deposition of Cr on Zircaloy-4 was successfully developed. A database of binary phase diagrams was constructed for the search for Cr-based dilute alloys. The synthesis and corrosion behaviors were done to deduce the candidate solute elements and their composition. An in-situ mechanical test system with AE signal acquisition and image observation was developed to evaluate mechanical behavior. The advanced expansion-due-to-compression (A-EDC) method was developed to derive mechanical strength in the hoop direction of cladding tubes.

[Corrosion and hydrogen effect] Hydrogen generation associated with corrosion reactions was clarified by experiments and first-principles calculations. The stabilities of adsorbed water molecules on Cr and its oxide surfaces were calculated to generate oxygen atoms and hydrogen molecules. The effect of residual oxygen in the environment on hydrogen formation was also clarified.

[Irradiation effect] An ion accelerator with a terminal voltage of 200kV was introduced to perform dual-beam irradiation with a Tandetron accelerator at HIT, The University of Tokyo. Cr-coated zircaloy was irradiated with H or He ions at elevated temperatures, followed by nano-hardness tests and SEM/EDS and FIB/TEM observations.

*Keywords: Nuclear fuel cladding, Accident tolerant fuel, Cr coating, Zircaloy*

# The development of interatomic potentials and simulations of primary radiation damage for vanadium alloys

**Huiqiu Deng**[1], Rongyang Qiu[2], Yangchun Chen[3]

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## Abstract

Vanadium (V)-based materials are considered candidates for future fusion reactor structures because of their excellent properties. However, the irradiation properties and mechanisms of V alloys remain unclear due to experimental limitations of irradiation and the lack of efficient and accurate correlation potentials required for multi-scale simulations. In this work, the Finnes-Sinclair-form alloy potentials for V-Ti-Ta-Nb were developed. The constructed potentials accurately describe the point defect properties as well as the enthalpy of formation, elastic constants of the binary alloy. The primary irradiation damage and the long-time evolution of defects in V, V-5Ti-5Ta alloy, V-Ti-Ta MEA and V-Ti-Ta-Nb HEA were then investigated by molecular dynamics methods using the developed potential. It was found that the fraction of defect clustering, defect cluster size and the number of dislocation loops of V-Ti-Ta MEA and V-Ti-Ta-Nb HEA were lower after the collision cascade compared to pure V and V-5Ti-5Ta alloys. This study expands the library of potentials for the V alloys and shows that the V-Ti-Ta MEA and the V-Ti-Ta-Nb HEA exhibit superior irradiation resistance than the conventional V-5Ti-5Ta alloy and pure V.

*Keywords: high-entropy alloys; interatomic interaction potential; collisional cascade*

# Distinct irradiation resistance mechanisms of high entropy alloys

Chenyang Lu [1*], Tan Shi[1], Zhengxiong Su[1], Ping Zhang[1]

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**Abstract**

High entropy alloys (HEAs) have demonstrated excellent mechanical properties and damage resistance owing to their unique features of lattice distortion, sluggish diffusion, high-entropy effect and cocktail effect. The great radiation resistance behavior of HEAs derives from the unconventional kinetic evolution of radiation defects from generation to long-term growth. This presentation will introduce a thorough investigation into the irradiation resistance mechanisms of FCC and BCC HEAs. The FCC HEAs, typically composed by Ni, Co, Fe, Cr and Mn, show significantly improved radiation resistance compared to low entropy counterparts. It is found that the evolution of irradiation defects including dislocation loops and voids can be delayed with tuning the alloy compositional complexity. Latest study reveals that unique short-range orders (SROs) structure in HEAs provides a novel strategy to modulate defect annihilation and evolution by tuning chemical and structural heterogeneities. The BCC HEAs, typically composed by refractory elements of Nb, Mo, Hf, Ta and W, are promising for higher temperature application due to their high strength over wide operating temperature ranges. Latest study shows that severe lattice distortion and irregular energy landscape in the NbZrTi alloy result in distinct point defect behaviors. The structural instability of defect clusters and closer mobilities between vacancy and interstitial enhance irradiation tolerance by promoting point defect annihilation and recombination. The exceptional mechanisms of defect evolution in HEAs shed the new light on developing radiation-tolerant materials for advanced fission and fusion reactors.

**Chenyang Lu, chenylu@xjtu.edu.cn**

*Keywords: High entropy alloys; irradiation effects; dislocation loops; short-range order; void swelling*

# Study on Phase Stability and Mechanical Properties in Mn-Ni-Si Model Alloys under Thermal Aging and Irradiation

**Xinrun Chen**[1], Ba Vu Chinh NGUYEN[2], Zhehuang Zhang[3],Tatsuya Suzuki[4], Kenta Murakami[5]

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## Abstract

$Mn_6Ni_{16}Si_7$ intermetallic compounds so called G-phase has been studied in diverse field because it has excellent magnetic inhibition property and superconductivity. In nuclear material field, this phase and its precursors are known as secondary phases precipitated in neutron-irradiated steels, and is considered to be the main cause of embrittlement in low-alloyed reactor pressure vessel steels under long-term operation. However, the Mn-Ni-Si precipitates in nuclear structural materials is very small, such as 3 nm, and their own stability and mechanical properties is unclear though it has been assumed for the multi-scale simulations.This study is utilized to supple some thermodynamic information and phase equilibrium data of G phase in Mn-Ni-Si system and give some advice to the formation mechanism under radiation.

Two Mn-Ni-Si model alloys (composed of 6Mn-16Ni-7Si and 30Mn-58Ni-12Si) were fabricated by vacuum induced melting, were cut into plates, and were thermal aged at 1273K in vacuum condition for 10 days. 6Mn-16Ni-7Si plate was irradiated by 2.8Mev $Fe^{2+}$ ion irradiation at 1~2 dpa (displacement per atom) at 573 K.

Multiple phases containing all Mn-Ni-Si were observed in both model alloys. The formation of G phase in both alloys after thermal aging was confirmed by XRD and SEM-EDS. Meanwhile, ratio of phases may be changed after thermal ageing. Young modulus measured by instrumentation indentation tests in G phase was 224.8(±6.6) GPa. Thermodynamic stability of G phase in each state will be simulated by CALPHAD lately.

*Keywords: G phase($Mn_6Ni_{16}Si_7$), Mn-Ni-Si alloys, Phase transition,Thermal aging,Irradiation*

# Technical **Oral Session _ Session 2**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 2 (H2)** **14:00 - 15:25, Nov. 20**

Chair : Haein Yim (Sookmyung Women's University) 303B, 3F

14:00-14:30 **K-H0582** **[Keynote] Study on Static and Dynamic Magnetic Properties of Amorphous Submicron Fe-B Spherical Particles**
Yasushi Endo (Tohoku University, Japan)

14:30-14:50 **I-H1184** **[Invited] THz Spin Dynamics in Ferromagnetic Thin Multilayers**
Dong-Hyun Kim (Chungbuk National University, Korea)

14:50-15:10 **I-H1004** **[Invited] A supercooling solidification technique to achieve Fe-based soft magnetic alloys with enhanced performance**
Chen Wu (Zhejiang University, China)

15:10-15:25 **O-H0986** **Storage and loss characterisations of electromagnetic energy in thin film of the Fe20Ni80 alloy**
Desheng Xue (Lanzhou University, China)

# Study on Static and Dynamic Magnetic Properties of Amorphous Submicron Fe-B Spherical Particles

**Yasushi Endo**

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## Abstract

Soft magnetic metal particles have a high potential as high-frequency magnetic cores because of their high resistivity and saturation magnetization. In particular, the submicron sized particles synthesized by chemical reduction of solutions have attracted much attention from fundamental point of view. However, little attention has been paid to their magnetic properties such as magnetic softness, high permeability and so on for high-frequency applications. Until now, we reported magnetic softness and permeability of amorphous Fe-B-P particles with the diameter of 0.3 μm synthesized by a chemical process. Herein, we focused on amorphous Fe-B spherical particles with various submicron sizes synthesized by chemical preparation in an aqueous method, investigated static and dynamic magnetic properties of these particles in detail, and further discussed the influence of submicron size on their properties.

The saturation magnetization and remanence ratio of the particles does not depend on the median size, and their values are 135-150 emu/g and approximately 0.02-0.05, respectively. The coercivity of the particles linearly decreases with the increase of the median size. In addition, each broad ferromagnetic resonance peak appears in the several GHz range, which might be ascribed to dipole-dipole interaction between particles and/or effective diamagnetic field. Therefore, these results suggest that the amorphous submicron Fe-B spherical particles possess the good magnetic softness and are one of the candidates as soft magnetic materials for next generation high-frequency applications.

Acknowledgement: This work was supported in part by MEXT Program Grant Number JPJ009777 and Grant Number JPMXP1122715503, CSIS, CSRN, and CIES of Tohoku University.

*Keywords: Submicron particles, Fe-B, Coercivity, Ferromagnetic resonance, Permeability*

# THz Spin Dynamics in Ferromagnetic Thin Multilayers

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## Abstract

Spin dynamics over wide timescales from ultraslow to ultrafast regions has attracted much attention due to possible application for ultrafast-operating and long-term stable spintronic devices. Ultrafast spin dynamics is inevitably involved with THz emission behavior due to the matching timescale of sub-ps magnetoelectric interaction. In this talk, we report our observation of THz emission dynamics for Co-based multilayers, resulted from ultrafast sub-ps spin dynamic phenomena such as inverse spin Hall effect and inverse Rasha Edelstein effect. Interface effect between ferromagnetic/nonmagnetic layers will be analyzed with consideration of reflection and attenuation of generated THz wave. Few examples of THz emission from exchange-biased systems will be also discussed.

*Keywords:* THz emission, Ultrafast spin dynamics

# A supercooling solidification technique to achieve Fe-based soft magnetic alloys with enhanced performance

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**Abstract**

Soft magnetic alloys are technologically important for the conversion and transmission of information and energy in fields such as telecommunication, information and energy. It is however, challenging to simultaneously optimize the saturation magnetization and coercivity. Here an undercooling solidification strategy has been proposed to achieve coordinated control of composition and microstructure in Fe-based soft magnetic alloys. For the designed FeSiCo system, it has been found that increased undercooling degree leads to both grain refinement and the formation of granular precipitates consisting of disordered α-Fe (Co) and B2 phase of the FeCo at the grain boundaries (GBs). Meanwhile, the domain structure transforms from the spike and lancet domains to refined 180° domains. The ferromagnetic precipitates at the GBs enhance the motions of magnetic domain walls during the magnetization process via the exchange coupling interaction, giving rise to simultaneously improved magnetization and coercivity. As such the work provides a new pathway to tune microstructures of soft magnetic alloys with enhanced performance.

*Keywords: Soft magnetic alloys; Undercooling solidification; Microstructure; Magnetic domains; Magnetic properties*

# Storage and loss characterisations of electromagnetic energy in thin film of the $Fe_{20}Ni_{80}$ alloy

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## Abstract

High storage density and low power loss of electromagnetic energy are the key performance of soft magnetic materials. However, the huge loss of soft metallic magnetic materials restricts their application in MHz frequency range in which the wide bandgap semiconductors can release full potential of efficient power conversion. Here, we introduce characteristic parameters $S = \chi_i \omega_r$ and $L = \chi''_{max} \Delta\omega$ to describe the energy storage and loss level of soft magnetic materials, respectively, where $\chi_i$ is the initial susceptibility, $\omega_r$ is the resonance frequency, $\chi''_{max}$ is the maximum of imaginary susceptibility, and $\Delta\omega$ is the half width of imaginary part. Based on Landau-Lifshits-Gilbert equation, without eddy current $S = L = \gamma M_s \sqrt{1 + H_\perp / H_\parallel}$ is derived within a general anisotropic free energy model, where $\gamma$ is the gyromagnetic ratio, $M_s$ is the saturation magnetization, and $H_\perp$ and $H_\parallel$ are the effective magnetic fields perpendicular and parallel to the easy magnetization plane, respectively. On the other hand, with eddy current $S = \gamma M_s \sqrt{1 + H_\perp / H_\parallel} > L$ is observed in $Fe_{20}Ni_{80}$ film, and the dependence of damping factor $\alpha$ on $L$ satisfies a linear scale as $L = (P\alpha + N)\gamma M_s \sqrt{1 + H_\perp / H_\parallel}$, where both $P$ and $N$ are constant parameters. Hence, our findings provide an new angle of view to understand the relation between energy storage and loss level of soft metallic magnetic materials.

*Keywords: Energy storage, Loss level, Soft metallic magnetic composites, Fe-Ni film*

# Technical **Oral Session _ Session 2**

## **Symposium I :** Biomaterials and Soft Materials and their Application

**Biomaterials and Soft Materials and their Application 2 (I2)** **14:00 - 15:40, Nov. 20**

Chair : Tae Hyeon Nam (Gyeongsang National University) 400, 4F
Yusuke TSUTSUMI (National Institute For Materials Science)

14:00-14:30 **K-I0262** **[Keynote] Decellularized biological tissues as new biomaterials**
Akio KISHIDA (Tokyo Medical and Dental University, Japan)

14:30-14:50 **I-I1102** **[Invited] Smart Polymer Technologies for Global Health**
Mitsuhiro EBARA (National Institute for Materials Science, Japan)

14:50-15:10 **I-I0505** **[Invited] Simultaneous 3D Printing Technology of Calcium Deficient Hydroxyapatite of Osteoblast Cells in a Hydrogel Bath System**
Hui-Suk YUN (Korea Institute of Materials Science, Korea)

15:10-15:40 **K-I1127** **[Keynote] Applying multiple surface treatments to regulate bone remodeling of titanium dental implants**
Her-Hsiung Huang (National Yang Ming Chiao Tung University, Taiwan)

# Decellularized biological tissues as new biomaterials

**Akio Kishida**

Department of Material-based Medical Engineering, Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo 101-0062, JAPAN
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## Abstract

Biological tissues, especially autologous tissues, are one of the ideal materials for tissue regeneration. Decellularized tissue is anticipated as a second option since its structure and mechanical properties are maintained. Decellularized human tissues, such as heart valves, blood vessels, and dermis, are already in clinical application. Decellularized tissues from xenogeneic animals, such as pigs and cows, are also currently being studied. Washing with detergent is the most common method of preparing these decellularized tissues, but it sometimes causes problems. We have developed a new decellularization method using high hydrostatic pressure (HHP). The effect of HHP pressurization is independent of tissue size because tissues set in the pressurized chamber are processed uniformly. We have reported HHP decellularization of heart valves, blood vessels, bone, and cornea. Furthermore, HHP treatment has been reported to have the ability to eliminate bacteria and inactivate viruses. Therefore, HHP treatment is also expected to be a sterilization method. We have been studying the efficient decellularization and recellularization of biological tissues to create biological scaffolds that do not lose their structural and biomechanical properties. I will report recent research results on tissue engineering using HHP decellularized tissues.

*Keywords: Decellularized tissue, Tissue engineering, High hydrostatic pressure, Detergent treatment.*

# Smart Polymer Technologies for Global Health

**Mitsuhiro Ebara**

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## Abstract

Our research group have been developing various types of "smart polymers". Smart polymer is the general term for polymers that have a property that will turn on and off in response to an external stimulus. Examples of such include temperature-responsive polymers, light-responsive polymers, and pH-responsive polymers. In addition to stimuli-responsive polymers, more recently smart polymers have been developed with shape memory, self-repairing capabilities, and biodegradability. If it is possible to apply such smart properties in the medical field, the we expect that this approach might contribute in part to medical treatments that can be received by anyone without being influenced by the infrastructure. Some examples are summarized in Fig.1. Temperature-nanofiber meshes have been developing towards cancer therapy1). (a) The nanofibers are composed of temperature-responsive polymers, magnetic nanoparticles (MNPs), and anticancer drug. Upon the application of alternating magnetic field, the MNPs generates heat and induces drug release from the fibers. (b) Temperature-responsive polymers have been also applied for the enrichment of biomarkers for infectious diseases. We have successfully increased the limit of detection of lateral flow immunoassay for COVID-192). (c) We have also been developing a wearable hemodialysis system. We have been developing zeolite-composite nanofiber meshes for the removal of various types of uremic toxin from kidney failure patients3). We expect that such smart polymer technologies can contribute to the improvement of global health in the future.

*Keywords: Smart Polymers, Diagnosis, Drug Delivery, Shape-memory, Inflammation*

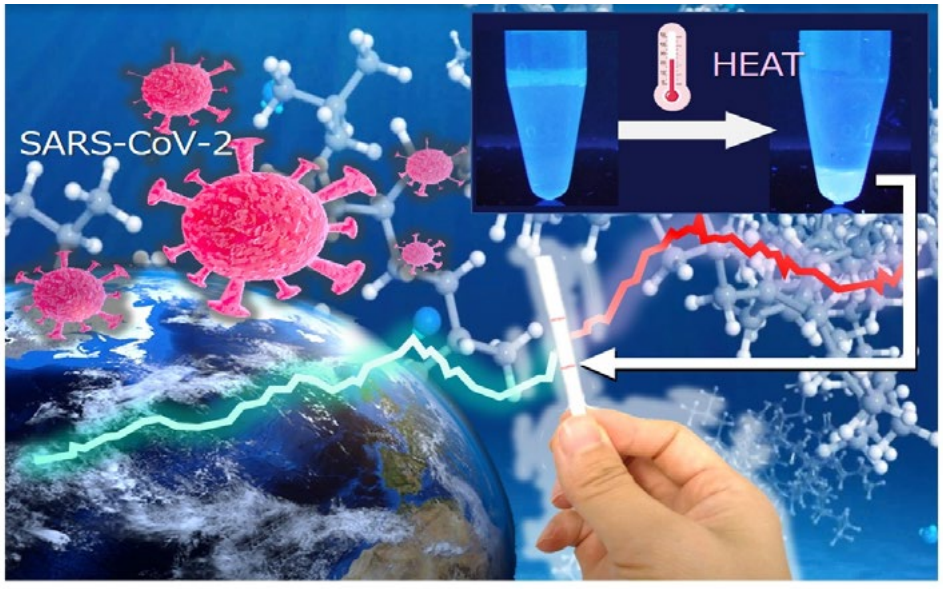



Figure 1 Smart enrichment strategy for SARS-CoV-2 using temperature-responsive polymers.

# Simultaneous 3D printing Technology of Calcium Deficient Hydroxyapatite and Osteoblast Cells in a Hydrogel Bath System

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Material extrusion (ME) is one of representative 3D printing processes in which material is selectively dispensed through a nozzle. ME processes are widely applied to produce 3D porous bioceramic scaffolds in bone tissue regeneration. The ceramic scaffolds are generally sintered after control 3D structures by ME process to achieve the desired mechanical properties. However, the sintering process often leads to shortcomings in biofunctional performance of ceramic scaffolds because functional materials such as biomolecules and drugs are easily denatured by heat and therefore cannot simultaneously print with ceramics. Our group is the first to suggest a novel ME process for creation of bioceramic scaffolds without sintering, to enhance the biofunctionality of scaffolds while retaining mechanical strength. Mechanical stability of the bioceramic scaffold was achieved by adapting a self-setting reaction after ME process rather than using a sintering process. Both final crystal state and biodegradability of scaffolds were also controlled by adjusting self-setting reaction. This process could be applied to fabricate various types of bioceramic scaffolds with biofunctional materials, such as osteoblast cells, drugs, biomarkers, and proteins, thereby providing highly functional scaffolds for effective bone tissue regeneration. Moreover, it can be applied for the simultaneous 3D printing of hydrogel-based live-cells and bioceramics. Self-standing 3D ceramic structures can be fabricated without any supporting structure as the process is performed in a gel-bath system. We believe that these new technologies may expand application markets of ceramic 3D printing technologies in biomedical fields.

# Applying multiple surface treatments to regulate bone remodeling of titanium dental implants

**Her-Hsiung Huang**

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## Abstract

Despite the widespread use of titanium for dental implants, some patients with poor bone quality need more time to heal and integrate the implant into the bone. The aim of this study was to modulate bone remodeling by altering the surface characters of titanium implants, i.e., to shorten the bone healing time required in patients with low bone quality, thus achieving rapid and good osseointegration. In vitro experiments have confirmed that titanium surfaces treated with a mixture of sandblasting/acid-etching/alkaline treatment produced a three-dimensional reticulated pore structure mimicking the appearance of the extracellular matrix (ECM). Type I collagen was then cross-linked with the natural crosslinker, epigallocatechin-3-gallate (EGCG), and immobilized on the titanium surface. The collagen-immobilized ECM-like titanium surface simultaneously promoted osteogenesis and inhibited osteoclast activity in vitro. The proposed multiple surface treatments have been successfully applied to commercial screw-type titanium dental implants. In vivo studies utilizing a rat model are currently underway. It is expected that in vivo experiments will demonstrate that this multiple surface treatment process for titanium dental implants can promote osseointegration in patients with poor bone quality by regulating bone remodeling.

*Keywords: Surface treatment; epigallocatechin-3-gallate (EGCG); type I collagen; osteogenesis, osteoclastogenesis.*

# Technical **Oral Session _ Session 2**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 2** **14:00 - 15:20, Nov. 20**

**Chair :** Dong-Ik Kim (Korea Institute of Science and Technology) 201B, 2F

14:00-14:30 **K-J1** **[Keynote]**
Kazuto ARAKAWA (Shimane University, Japan)

14:30-15:00 **K-J0171** **[Keynote] Role of dislocation movement on the phase transformation of metastable precipitate to stable phase in the steels**
YOON-UK HEO (Pohang University of Science and Technology, Korea)

15:00-15:20 **I-J0799** **[Invited] Direct observation of quadrupolar strain fields forming a shear band in metallic glasses using 4D-STEM**
Sangjun Kang (Karlsruhe Institute of Technology & Technical University Darmstadt, Germany)

# Role of dislocation movement on the phase transformation of metastable precipitate to stable phase in the steels

**Yoon-Uk Heo**[1*], T. T. T. Trang[2], Dongwon Lee[3], Dong-Hyun Kim[4]

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## Abstract

Phase transformation of metastable precipitate to stable phase in various steels was studied by transmission electron microscopy (TEM). TEM results revealed the detailed transition steps during the transformation. The changes in crystal structure and chemical composition were investigated using high-resolution TEM, high-angle annular dark field scanning TEM, EDS, and EELS analyses. Although the compositional change stage varies depending on the alloy system, the metastable precipitate is transformed into other phases by dislocation movement in the metastable precipitate. Schockely partial dislocation glide or Frank dislocation climb-up changed the crystal structure of the metastable precipitates. The role of dislocation movement on the phase transformation of metastable precipitate to stable phase is discussed. Finally, the effect of the metastable to stable phase transformation of precipitate on the mechanical property is further discussed.

*Keywords: Phase transformation, Dislocation climb, Twinning, Metastable precipitate*

# Direct observation of quadrupolar strain fields forming a shear band in metallic glasses using 4D-STEM

**Sangjun Kang**[1], Xiaoke Mu[2], Wang Di[3], Christian Minnert[4], Karsten Durst[5], Christian Kübel[6]

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## Abstract

In this work [1], we have successfully addressed the long-standing challenge of experimentally imaging the atomic packing structure and local strain in amorphous materials using 4-dimensional scanning transmission electron microscopy (4D-STEM). We capture 2D images of local diffraction patterns over a 2D grid by systematically scanning the probe across the region of interest. The local strain is quantified by analyzing the elliptical deviation present in each diffraction pattern, with the principal strains determined from the long and short axes of the ellipse. By algebraically transforming the principal strains into loading coordinates, we obtain the strain tensor. Furthermore, we perform a pair distribution function (PDF) analysis as a structural descriptor based on the 4D-STEM dataset, enabling us to analyze the local atomic structure of metallic glasses. Consequently, the 4D-STEM technique offers a comprehensive visualization of the nanoscale strain field alongside valuable atomic structure information.

To illustrate the capabilities of our approach, we investigate a deformed Fe-based metallic glass ribbon as a case study [2]. Our observations reveal residual strain fields localized at inclusions within the metallic glass. This visualization provides the first experimental evidence of Eshelby-like inclusions surrounded by quadrupolar strain fields aligned along a shear band in deformed metallic glasses. As a result, we gain new insights into the mechanisms governing shear band formation in metallic glasses. It is expected that our novel method will open up new avenues for extensive research aimed at addressing various inquiries concerning amorphous materials.

*Keywords: 4D-STEM, Eshelby inclusions, metallic glass, shear bands, strain fields*

## Reference

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[2] C. Schuh, T. Hufnagel, U. Ramamurty, Mechanical behavior of amorphous alloys, *Acta Materialia*, 55, 2007, 4067-4109.

# Technical **Oral Session _ Session 2**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 2 (K2)** **14:00 - 15:30, Nov. 20**

**Chair :** Wan Chuck WOO (Korea Atomic Energy Research Institute) Samda Hall B, 3F

14:00-14:30 **K-K0452** **[Keynote] Opportunities for FCC High/Medium-Entropy Alloys**
Koichi Tsuchiya (NIMS, Japan)

14:30-14:50 **I-K0698** **[Invited] Cost-Effective High-Entropy Alloys with Superior Properties**
Yin Yu (University of Queensland, Australia)

14:50-15:10 **I-K1035** **[Invited] Nanostructure engineering toward high-performance multiple principle alloys**
Xianghai An (The University of Sydney, Australia)

15:10-15:30 **I-K0999** **[Invited] Advancements of eutectic high-entropy alloys**
Yiping Lu (Dalian University of Technology, China)

# Opportunities for FCC High/Medium-Entropy Alloys

**Koichi Tsuchiya**[1]

[1] Research Center for Structural Materials, National Institute for Materials Science, Tsukuba, 305-0047, Japan

## Abstract

FCC High- or Medium- entropy alloys attracted much attention after the discovery of CrMnFeCoNi (Cantor alloy) due to the superb strength-elongation balance even at cryogenic temperatures. Such enhanced mechanical properties can be attributed to low stacking fault energy and/or to the metastability of the FCC phase. The present talk elucidates the effect of FCC-HCP phase stability on deformation as well as the fatigue behavior in FCC high-/medium-entropy alloys.

Gibbs free energy was evaluated for FCC and HCP phase for $Cr_{20}Mn_{20}Fe_{20}Co_{40-x}Ni_x$ alloys by the Calphad approach. The results indicated that Co content stabilizes HCP phase at room temperature. The 10Ni and 15Ni alloys exhibited fairly good strength-ductility balance due to TRIP effect and TWIP effect, respectively.

Aiming for the application to medical devices, $Co_{50-x}Cr_{20}Mo_{10}Ni_{20+x}$ ($x$ = 0–15) MEAs were designed based also on the FCC-HCP phase stability. Room temperature tensile tests revealed a high work-hardening rate and good strength–elongation balance of the alloys. XRD and EBSD analysis revealed that the dominant deformation modes gradually shift from the FCC-HCP transformation to deformation twinning with the Ni content. It should be noted that HCP phase and twins coexist in the $x$ = 3–9 alloys. The low cycle fatigue (LCF) behavior was investigated with a total strain amplitude of 0.02. The highest LCF lives were observed for the $x$ = 6 alloy (6537 cycles). They are much higher than those of MP35N or L605. These findings suggests that the formation of ε-twin bundles may be an important factor to obtain high LCF resistance. Microstructures and mechanical properties of tubes and wires made of the MEA alloys as well as the property of a proto type stent will also be reported.

*Keywords: TRIP, TWIP, martensitic transformation, stacking fault energy*

# Cost-Effective High-Entropy Alloys with Superior Properties

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## Abstract

High-entropy alloys (HEAs) possess a multi-component characteristic that often results in high material costs, posing a challenge to their widespread industrial applications. Therefore, it is crucial to develop cost-effective HEAs that offer exceptional performance and comprehensive properties. In this study, we propose innovative strategies involving composition design and microstructure control to achieve cost-effective HEAs with superior properties. The newly developed FeNiCrMo-based HEAs demonstrate remarkable comprehensive properties. At room temperature, they exhibit a yield strength surpassing 1 GPa along with an elongation of approximately 13%. Moreover, these alloys showcase exceptional tensile strength, exceeding 1.4 GPa, and an elongation of 20% at liquid nitrogen temperature. Notably, their oxidation resistance at high temperatures (1200 °C) surpasses that of the commercially available superalloy Inconel 625, while their corrosion resistance outperforms that of the widely used 316L stainless steel. Furthermore, the wear resistance of the FeNiCrMoTiC high-entropy composite, derived from the FeNiCrMo HEAs, exceeds even that of the commercial high-chromium cast iron. This characteristic highlights its immense potential for applications in extreme environments characterized by abrasion, corrosion, and oxidation. These findings present a viable solution for utilizing high-entropy alloys in challenging conditions.

*Keywords: High entropy alloys; Composition design; Microstructure; Properties*

# Nanostructure engineering toward high-performance multiple principle alloys

**Xianghai An**

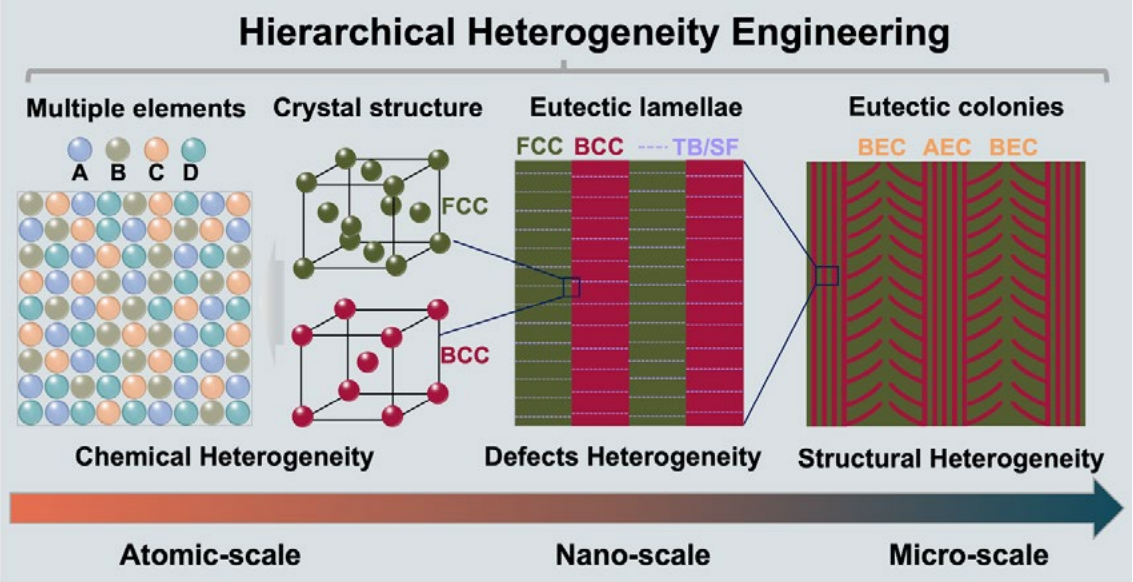
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## Abstract

High-performance alloys, playing critical roles in the performance and lifespan of many engineering components, are the backbone of decarbonising innovations in manufacturing, infrastructure, and transportation. A vital requirement for all structural materials is that they are strong, ductile, durable, and damage tolerant. However, these characteristics cannot currently be obtained simultaneously. After decades of exploration, many engineering alloys seem to have approached their performance limits. The fundamental tenet in materials science is that a material's properties are dictated by its compositions and nanostructures. Recently, by mixing three or more major elements in massive quantities (see the figure), a new paradigm of multiprincipal element alloys (MPEA), also well known as high-entropy alloys (HEA), has been recently exploited, enabling a vast compositional space previously inaccessible and presenting a multitude of new opportunities for novel deformation mechanisms and then materials properties. A delicate incorporation of local chemical and structural heterogeneities spanning multiple length scales could greatly push the boundaries of materials properties beyond current benchmark ranges. In this presentation, I will discuss the distinct deformation mechanisms at nano-and micro-scale, and the superior mechanical properties of MPEAs/HEAs with local chemical and nanostructural heterogeneities.

1. **X.H. An***. *Structural Hierarchy defeats alloy cracking.* ***Science*** 373 (2021) 857-858.
2. H. Wang, D.K. Chen, **X.H. An***, Y. Zhang, S.J. Sun, Y.Z. Tian, Z.F. Zhang, A.G. Wang, J.Q. Liu, M. Song, S.P. Ringer, T. Zhu*, X.Z. Liao*.*Deformation-induced crystalline-to-amorphous phase transformation in a CrMnFeCoNi high-entropy alloy.****Science Advances*** 7 (2021) eabe3105.
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Figures: The schematics represent the multilevel hierarchy of chemical and nanostructural heterogeneities towards high-performance alloys.[1]

*Keywords:* multiprincipal element alloys, hierarchical nanostructure heterogeneities, *mechanical properties, deformation mechanisms.*

# Advancements of eutectic high-entropy alloys

**Yiping Lu[1], Tingju Li[1], Tongmin Wang[1], Mingliang Wang[1], Shudao Wang[1], Tianxin Li[1], Dingfeng Xu[1]**

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## Abstract

Eutectic High-entropy alloys (EHEAs) have been proposed since 2014. Because of their excellent comprehensive mechanical properties and good casting fluidity, they are one of the most potential High-entropy alloys for industrial application. At present, they have become a hot spot in the research field of High-entropy alloy. This report summarized the latest research progress of our team, introduced the phase composition, microstructures, mechanical properties, and composition design methods of EHEA in detail, and finally pointed out the challenges faced by EHEA and looked forward to their future development.

*Keywords: Eutectic High-entropy alloys, phase composition, microstructures, mechanical properties*

# Technical **Oral Session _ Session 2**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 2 (L2)** **14:00 - 15:35, Nov. 20**

Chair : Hansang Kwon (Pukyong National University), Seungchan Cho (Korea Institute of Materials Science) 202B, 2F

14:30-14:50 **I-L1062** **[Invited] In situ synthesis of Al-AlN Composites by arc plasma-induced accelerated volume nitridation**
Je In Lee (Pusan National University, Korea)

14:50-15:05 **O-L0907** **Microstructure regulation and hot compression behaviour of network structured TiBw/Ti65 composites**
Shaocong Xiong (Harbin Institute of Technology, China)

15:05-15:20 **O-L0888** **Microstructure and properties of metal matrix composites prepared by accumulative roll-compositing**
Qingsong Me (Wuhan University, China)

15:20-15:35 **O-L0879** **Wire filled tungsten argon arc welding of titanium matrix composites**
Jie Zhang (Harbin Institute of Technology, China)

# In situ synthesis of Al-AlN Composites by arc plasma-induced accelerated volume nitridation

Su Jin Jung[1], **Je In Lee[1]**

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## Abstract

Thermal conduction and thermal expansion behaviors of heat sink materials are crucial for microelectronic packaging. High thermal conductivity (TC) is required to remove the heat generated on component parts, and a low coefficient of thermal expansion (CTE) is needed to reduce thermal stress and improve dimensional stability. In the present study, we report a new type of aluminum nitride (AlN) reinforced aluminum matrix composites. The novel composites are fabricated by in situ reaction between liquid aluminum and nitrogen gas through arc melting. Our results show that a volume fraction of AlN reinforcements can be increased up to around 40% depending on the nitridation reaction time. Our results propose that the in situ Al-AlN composites could exhibit an attractive combination of high TC and low CTE, which is highly desirable for heat sink materials.

**Keywords:** Composite, Aluminum, Aluminum nitride (AlN), Thermal conductivity, Thermal expansivity

# Microstructure regulation and hot compression behaviour of network structured TiBw/Ti65 composites

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**Abstract**

In response to the requirements of lightweight, heat-resistant, and high-strength materials for key components in the next-generation spacecraft engines, this study selected the near α-phase Ti65 alloy, capable of operating at temperatures up to 650℃, as the matrix material for the composite. TiBw/Ti65 composite materials with different network structure parameters (including reinforcement phase content and network size) have been successfully prepared through low-energy ball milling and hot pressing sintering techniques. The influence patterns of network structure parameters on the microstructure and mechanical properties of composite materials were investigated, while also assessing the thermoforming capability of the composite materials. The experimental results indicated that the introduction of TiB whiskers transformed the matrix from a Widmanstatten structure to a basket-weave structure. Microscale TiB whiskers at the network boundaries and nanoscale silicide at the phase interfaces formed a dual-scale two-level network structure. Furthermore, an increase in TiBw content leaded to higher tensile strength but reduced elongation at room temperature. As the network size decreased, both the tensile strength and elongation of the composite material initially increased and then decreased. Moreover, the maximum tensile strengths of the composite material at 600°C, 700°C, and 800°C were 823MPa, 615MPa, and 349MPa, respectively, representing improvements of 36%, 18%, and 14% compared to Ti65 alloy. Finally, the activation energy for the thermal deformation of the composite material was calculated to be 321.57kJ/mol, indicating that the thermal deformation was predominantly governed by dislocation motion. Additionally, the thermal processing map displayed the suitable processing window as 1070°C-1100°C and $1s^{-1}$-$0.1s^{-1}$.

*Keywords: high-temperature titanium matrix composites, network architecture, tensile properties, hot compression*



**Presenting author:** **Shaocong Xiong**
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**Symposium L: Composite, Coating and Hetero-Materials**

# Microstructure and properties of metal matrix composites prepared by accumulative roll-compositing

**Qingsong Mei**[1], Guodong Zhang[1], Juying Li[3]

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## Abstract

The distribution of nano reinforcements in the matrix is one of the key factors affecting the properties of metal matrix composites (MMCs). In our studies, Al and Cu matrix composites reinforced by different types of nano reinforcements were prepared by accumulative roll-compositing (ARC) process with high rolling cycles. The dispersion and the in-situ formation mechanisms of the nano reinforcements, formation of the uniform and heterogeneous microstructures, and the mechanical behaviors of the MMCs were investigated systematically. The results show that (1) ARC can enhance the dispersive distribution of nano reinforcements in the metal matrix; (2) ARC can enable the in situ formation of nano reinforcements, such as the delamination of graphene from graphite in the Cu/graphite composites; (3) ARC can facilitate the formation of heterogeneous microstructure in MMCs. (4) The ARC-prepared MMCs exhibit excellent comprehensive properties, with a synergistic strengthening effect in the MMCs with hybrid reinforcements. Our results show the high potential of the ARC process for preparation of MMCs with high performance by tailoring the compositing and distribution of nano reinforcements.

*Keywords: metal matrix composites; nano reinforcements; accumulative roll-compositing; synergistic strengthening; mechanical property*

# Wire filled tungsten argon arc welding of titanium matrix composites

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## Abstract

Titanium matrix composites have excellent properties such as lightweight and high strength. The TiBw/TA15 composite was prepared using vacuum hot pressing sintering technology, and was connected using wire filled tungsten argon arc welding technology. Microstructure and mechanical properties of the TiBw/TA15 composite argon arc welding joint was investigated. The welded joint is mainly composed of three areas: melting zone, heat affected zone, and base metal. The melting zone contains columnar crystal structure of lath and needle α' Martensite. The matrix of the heat affected zone is needle shaped α' Martensite and primary α phase. There is also a semi molten zone between the heat affected zone and the molten zone, in which the grains are relatively coarse and composed of a single α' phase. Compared to unfilled welding wire, filled welding wire can effectively reduce the hardness of the fusion zone and heat affected zone of the join, reducing the impact of stress concentration on the mechanical properties of the joint. When TA1 welding wire is filled and the welding current is 140A, the joint shows the highest tensile strength and has an elongation of 2.94%.

*Keywords: Titanium, metal matrix composites, gas tungsten arc weld, property.*

# Technical **Oral Session _ Session 2**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 2 (M2)** **14:00 - 15:20, Nov. 20**

**Chair :** Dong-Hyun Lee (Chungnam National University) 402, 4F

14:00-14:30 **K-M0849** **[Keynote] Augmenting Metal Properties via Cohesive Interfaces between Metallic and Nonmetallic Phases**
Seung Zeon Han (Korea Institute of Materials Science, Korea)

14:30-14:50 **I-M0342** **[Invited] Effect of Surface-nanostructure Layer Formed by Heavy Plastic Deformation Process on Rolling Contact Fatigue of Steels**
Yoshikazu Todaka (Toyohashi University of Technology, Japan)

14:50-15:05 **O-M0110** **Optimization of Strength-ductility synergy of gradient-structured Cu-Al-Zn via low temperature annealing**
Xinkun Zhu (Kunming University of Science and Technology, China)

15:05-15:20 **O-M0336** **Analysis of microstructure effects on strength and electrical conductivity of Cu/Nb nanolaminates**
Takayuki Shiraiwa (The University of Tokyo, Japan)

# Augmenting Metal Properties via Cohesive Interfaces between Metallic and Nonmetallic Phases

**Seung Zeon Han,** Eun-Ae Choi

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## Abstract

Interfaces are ubiquitous in all materials, including metals, and play a crucial role in either strengthening or degrading their properties. In precipitation-hardening alloys, the formation and growth of strengthening particles occur during specific thermomechanical treatments, commonly known as aging. During the early stages of aging, newly formed particles exhibit coherent crystallographic relationships with the matrix, and multiple interface relationships are observed at the interface between the precipitate and matrix planes. The variation in interface energy across different planes accounts for the differences in aspect ratio among particles.

From a strengthening mechanism perspective, achieving smaller particle sizes and reducing inter-particle distances are essential for increasing strength. The interface energy at each precipitate-matrix interface plane fundamentally influences the shape, size, and even distribution of particles.

In this study, we present successful research examples illustrating the enhancement of strength and other properties through the control of interface energy between precipitates and the alloy matrix. Additionally, we introduce an expanded concept of interface energy control by demonstrating a method to establish stable bonding between copper oxide and the copper matrix. Remarkably, the oxide-coated copper exhibits excellent resistance to fracture or delamination even after severe plastic deformation.

This research highlights the significance of interface energy manipulation in optimizing metal properties, paving the way for advanced material design and applications.

*Keywords: Interface, alloy matrix, precipitates, metal oxide, stable bonding*

# Effect of Surface-nanostructure Layer Formed by Heavy Plastic Deformation Process on Rolling Contact Fatigue of Steels

**Yoshikazu Todaka**[1], Nozomu Adachi[2], Yoshinori Shiihara[3], Masatoshi Mitsuhara[4], Atsushi Kubo[5], Yoshitaka Umeno[6]

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## Abstract

The effects of nanostructure (high-density of lattice defects) on the tribological and rolling contact fatigue behaviors were investigated in steels. In the nanostructured steels with high-density lattice defects (grain boundary, dislocation, etc.) produced by heavy plastic deformation processes, the stable tribological behavior with low friction coefficient was observed under oil lubrication, in comparison with the non-deformed steels having coarse grains. The rolling contact fatigue life was extended in the steels with the surface-nanostructure layer produced by the surface-nanostructured wearing (SNW) and the induction heating & quenching (IHQ). The improvement of rolling contact fatigue property is owing to not only the high hardness but also the reduction of friction coefficient during the roller pitting test followed by the suppression of dynamic tempering softening and the variation of stress distribution. These results indicate that the surface-nanostructure control of steels by heavy plastic deformation process and heat treatment is highly effective in improving the tribological and rolling contact fatigue properties.

Acknowledgment: This research was financially supported by JST “Collaborative Research Based on Industrial Demand: Heterogeneous Structure Control” (JPMJSK1511) and JSPS KAKENHI Grant-in-Aid for Scientific Research (B) & (A) (15H04155 & 22H00261). The induction heat treatments for sample preparation and the rolling contact fatigue tests were performed by NETUREN Co., Ltd. The authors gratefully acknowledge these supports.

*Keywords: rolling contact fatigue; friction coefficient; nanostructure; lattice defect; heavy plastic deformation.*

# Optimization of Strength-ductility synergy of gradient-structured Cu-Al-Zn via low temperature annealing

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**Abstract**

The surface deformation of the metals over long periods of time dramatically increases the strength while it drastically reducing the ductility. In this paper, Gradient-structured (GS) Cu-Al-Zn samples were produced by the surface mechanical attrition treatment (SMAT). Gradient-structured (GS) samples were annealed at 320℃ and 350℃ for 20 min to eliminate partially stored defects to optimize the strength-ductility synergy. Tensile results showed an increase in ductility for the short-annealed GS samples, but no significant reduction in strength, in which its synergetic strengthening effect and HDI stress were slightly reduced. The Digital Image Correlation (DIC) results showed that the strain distribution is more homogeneous in the short-annealed GS sample than that of GS samples. XRD and EBSD observations demonstrated that the high density of defects on the surface of GS sample were transformed into a low dislocation density microstructure, which can further improve the dislocation storage capability and therefore improve ductility.

*Keywords: Gradient Structure,* surface deformation, surface mechanical attrition treatment, *Strength, Ductility.*

# Analysis of microstructure effects on strength and electrical conductivity of Cu/Nb nanolaminates

**Takayuki Shiraiwa[1],** Koki Yasuda[1], Fabien Briffod[1], Manabu Enoki[1]

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**Abstract**

There has been considerable interest in metal-metal composites with nanoscale to microscale features owing to their high mechanical strength and electrical conductivity, which are crucial properties required for next-generation high-field generators and electrical devices. Although alloys often exhibit a trade-off relationship between electrical conductivity and tensile strength, metal/metal composites can enhance tensile strength while maintaining high electrical conductivity by controlling their phase distribution. Among these composites, copper/niobium (Cu/Nb) nanolaminates fabricated by accumulative roll bonding (ARB) has received attention in recent years due to its potential for practical applications in bulk material production.

The Cu/Nb nanolaminate has a microstructure of alternating stacks of Cu and Nb layers, and the spatial distribution of the two phases, including the volume fraction of each phase, layer thickness, and interface roughness, can be controlled by modifying the initial plate materials, rolling process, and subsequent heat treatment. However, determining the optimal process parameters for achieving a better balance between strength and conductivity through experimentation alone is challenging due to numerous controllable parameters. Therefore, in this study, we developed an accurate prediction model by finite element method (FEM) for both the tensile yield strength and electrical conductivity based on a limited amount of experimental data. Using this prediction model, repetitive virtual experiments were conducted to analyze the effects of the microstructural features on the mechanical and electrical properties. Subsequently, machine learning techniques were applied to the abundant data obtained from the calculations to quantitatively evaluate the linkage between microstructural features and materials properties.

*Keywords: Cu/Nb, Accumulative roll bonding, Finite element analysis, Electrical conductivity, Tensile strength*

# Technical **Oral Session _ Session 2**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 2 (N2)** **14:00 - 15:30, Nov. 20**

**Chair :** Irene Beyerlein (University of California Santa Barbara), Keonwook Kang (Yonsei University) **203, 2F**

14:00-14:30 **K-N0166** **[Keynote] Electronic and atomic structures of glide dislocations in inorganic semiconductors relevant to their light-illumination dependent mechanical behavior**
Katsuyuki MATSUNAGA (Nagoya University, Japan)

14:30-14:50 **I-N0216** **[Invited] A generalizable and interpretable deep learning model to improve the prediction accuracy of strain fields in grid composites**
Seunghwa Ryu (Korea Advanced Institute of Science and Technology, Korea)

14:50-15:10 **I-N0899** **[Invited] Research and development in microforming technology of metallic composites**
Zhengyi Jiang (University of Wollongong, Australia)

15:10-15:30 **I-N1159** **[Invited] Sequential Decision-making for Compositional Design of Multicomponent Alloys using Reinforcement Learning**
Dezhen Xue (Xi'an Jiaotong University, China)

# Electronic and atomic structures of glide dislocations in inorganic semiconductors relevant to their light-illumination dependent mechanical behavior

**Katsuyuki Matsunaga**

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**Abstract**

As reported experimentally, ZnS single crystals having the zincblende structure underwent extraordinarily large plastic deformation even at room temperature in complete darkness. In normal light-illumination environments, however, ZnS single crystals showed limited plastic deformation and finally fractured in a very brittle manner. It is thought that the above results may be due to changes in mobility of glide dislocations in ZnS due to light illumination. In order to clarify the mechanism at the electronic and atomic levels, DFT calculations of glide dislocations in ZnS were performed. It was found that glide dislocations in ZnS have excess electrostatic potentials localized at the cores and thus extra electrons and holes excited by light illumination can be favorably trapped at the dislocation cores. Such carrier trapping at the dislocation cores also accompanied atomic reconstruction, which may be closely related to the decreased dislocation mobilities under light illumination, namely hardening of ZnS. More details on characteristic electronic structures especially at the dislocation cores and the effect on the Peierls potentials will be discussed.

*Keywords: dislocation core, electronic structure, atomic reconstruction, carrier trapping, dislocation mobility*

# A generalizable and interpretable deep learning model to improve the prediction accuracy of strain fields in grid composites

Donggeun Park[1], Jiyoung Jung[2], Grace Gu[3], **Seunghwa Ryu**[4]

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**Abstract**

Recently, the design of grid composites with superior mechanical properties has gained significant attention as a testbed for deep neural network (DNN)-based optimization methods. However, current designed DNN architectures are not specifically tailored for grid composites and thus show weak generalizability in exploring unseen configurations that stem away from the training datasets. Here, a multiscale kernel neural network (MNet) is proposed that can efficiently predict the strain field within a grid composite subject to an external loading. Predicting the strain field of a composite is especially important when it comes to understanding how the material will behave under loading. MNet enables accurate predictions of the strain field for completely new configurations in unseen domain, with a reduced mean absolute percentage error (MAPE) by 50% compared to a benchmark, U-Net as current state-of-the arts DNN architectures. In addition, results showed that MNet maintained superb performances with less than one-third of dataset, and can be applied to grid composites larger than the composite configurations used for the initial training. By investigating the inference mechanisms from the kernels of multiple sizes, our work revealed that the MNet can efficiently extract various spatial correlations from the material distribution.

*Keywords: Deep neural networkInterpretable deep learningComposite designStrain fieldU-NetMaterial design.*

# Research and development in microforming technology of metallic composites

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## Abstract

Microforming technology is gaining more and more attention from modern industries due to the need for advanced high-precision micro products across various fields such as bio-medical, aerospace, microelectronics, and microelectromechanical systems (MEMS). Micromanufacturing techniques offer extensive application to a wide range of materials, enabling cost-effective production of complex metallic micro products with precise geometries, excellent dimensional tolerances, desired mechanical properties, and enhanced surface quality. As the demand for multifunctional micro products continues to rise, the utilisation of metallic composites in micromanufacturing has attracted significant attention and interest. Recent studies in advanced micromanufacturing have been undertaken on micro rolling of copper/SS304L composite to fabricate micro channels, micro deep drawing of aluminium/copper composite to produce micro cups, and micro flexible rolling of aluminium/copper composite to form ultrathin strips with longitudinal thickness variation. In the micro rolling of copper/SS304L composite, the effects of rolling reductions and velocities on the material deformation behaviours, microstructural evolution, mechanical properties, and processing mechanism were investigated. In the micro deep drawing of aluminium/copper composite, the drawability mechanism associated with different annealing temperatures was unveiled. For the case of micro flexible rolling of aluminium/copper composite, the effects of rolling reduction and annealing temperatures on the microstructure and tensile properties of rolled ultrathin strips were examined. Prospective research could focus on the utilisation of environmentally friendly water-based nanolubricants or coated graphene nanoplatelets combined with numerical simulation for the sustainable microforming technology of metallic composite products.

*Keywords: Microforming; Metallic composites; Nanolubrication; Numerical simulation; Micro products*

# Sequential Decision-making for Compositional Design of Multicomponent Alloys using Reinforcement Learning

**Dezhen Xue** [1]

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## Abstract

Current pool-based materials informatics tools to design compositions of multicomponent materials often depend on enumerating potential candidates in a large combinatorial space, resulting in a high computational cost and thereby a slow materials design process. We reformulate the design problem in terms of how compositions of components are selected using reinforcement learning, in which an agent makes decisions in a sequence. Online interactions are achieved by a surrogate model that is improved adaptively with experimental feedback. We demonstrate the strategy by designing a phase change multicomponent alloy ($Ti_{27.2}Ni_{47}Hf_{13.8}Zr_{12}$) with transformation enthalpy ($\Delta H$) 37.1 J/g from a space over $2\times10^8$ candidates, although the surrogate is initially trained on a compact dataset with 112 alloys. Further in-situ experiment indicates an origin of large lattice in-compatibility ($\lambda_2$ = 0.897) before and after phase transformation. Such an RL loop can be applied to the design of other materials, especially with a large search space and relatively few training samples.

*Keywords:Reinforcement learning; Active learning; High entropy alloys; Shape memory alloys.*

# Technical **Oral Session _ Session 2**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 2** — **14:00 - 15:20, Nov. 20**

**Chair :** Samane Maroufi (University of New South Wales) — 401, 4F

14:00-14:30 **K-O0895** **[Keynote] Strategies of the Japanese Steel Industry to Achieve Carbon Neutrality**
Takeo HOSHINO (The University of Tokyo, Japan)

14:30-14:50 **I-O0637** **[Invited] Environment induced degragation behavior of multicomponent alloys**
Hong Luo (University of Science and Technology Beijing, China)

14:50-15:05 **O-O0526** **Sensing of Multiphase Melts utilizing AC Electric Fields for Sustainable High-Temperature Metals Production**
Noritaka SAITO (Kyushu University, Japan)

15:05-15:20 **O-O0632** **Thermodynamics analysis of slag-metal reactions in steel refining considering interactions of tramp elements for green steelmaking**
Hideki Ono (University of Toyama, Japan)

# Title: Strategies of the Japanese Steel Industry to Achieve Carbon Neutrality

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## Abstract

We have entered an era in which achieving carbon neutrality has become a common goal for the world. All industries and companies must develop and implement strategies to reduce carbon dioxide emissions to zero by 2050. However, Basic materials such as steel, cement, and chemical materials are all difficult to electrify due to their production volumes that are orders of magnitude larger than those of other industrial products, their high energy input at the production stage, the high heat demand at high temperatures in the production process, and the inevitable emission of CO emissions achieving carbon neutrality is a challenging task.

In Japan, 40% of society's total CO2 emissions come from the industrial sector, of which the steel industry emits 160 million tons of CO2, accounting for about 40% of the industrial sector. Therefore, the carbon neutrality strategy of the steel industry is a significant key to achieving carbon neutrality for Japan. With support from the government's Green Innovation Strategy, Japanese blast furnace makers are taking on the challenge of developing system technology that combines blast furnace-based hydrogen reduction ironmaking process technology and carbon recycling technology, which is unprecedented worldwide. We are facing many technical and cost challenges. This presentation will introduce these efforts, present the status of recent studies, and discuss the direction of strategies that the global steel industry should take。

Keywords: Steel industry, carbon neutral strategy, blast furnace-based hydrogen reduction, carbon cycle

# Environment induced degragation behavior of multicomponent alloys

**Hong Luo**, Zhimin Pan, Xiaogang Li

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## Abstract

The corrosion and hydrogen-induced cracking of metal materials has plagued the engineering field for a long time and seriously threatened the service life and safety of the equipment. Over the years, scholars have been devoted to the research of hydrogen embrittlement (HE) mechanisms and HE resistant alloys. Multicomponent high-entropy alloys have unique design concepts and development characteristics. Starting from the principle of configurational entropy of the alloy system, a new alloy design perspective is proposed. They have excellent properties that many metal materials do not have, e.g., high hardness, high strength, heat resistance, corrosion resistance, etc., and are expected to be applied in aerospace, nuclear power, ocean, shipbuilding, and other industries. In this work, a variety of analysis and characterization methods were used to study the failure behavior and mechanism of several common high-entropy alloys in hydrogen environment. The results show that compared with ordinary alloys, high-entropy alloys have certain unique characteristics in terms of hydrogen cracking behavior and mechanism. Also, in addition to the conventional hydrogen-induced cracking mechanism, hydrogen-induced twinning has been found in high-entropy alloys. This discovery provides ideas for the design of new-type resistance to hydrogen embrittlement high-entropy alloys.

*Keywords: High entropy alloys; Face-centered cubic; Hydrogen-induced fracture*

# Sensing of Multiphase Melts utilizing AC Electric Fields for Sustainable High-Temperature Metals Production

**Noritaka Saito[1]**

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**Abstract**

In the steelmaking process, the slag by-product is not basically a homogeneous melt but a complex mixture of solids such as untreated CaO and coal, gases such as CO gas generated by the reaction between hot metal and slag, and liquids such as hot metal entrained by foaming slag. These fluids form a complex mixture of high-temperature fluids, and many problems are closely related to these fluids. The issue of non-negligible iron loss caused by the foaming slag produced in the hot metal pretreatment process, for example, is thought to be caused by a lack of understanding of the behavior of the second phase in the high-temperature slag matrix.

These second phases' presence significantly affects the control factors of high-temperature metallurgical processes, such as viscosity and thermal conductivity. From this perspective, our group has been detecting and quantifying solids and gases by applying an alternating electric field to molten slag. In addition to the above, I will present the results of high-precision measurement of the electrical conductivity of molten slag, which is indispensable for Electro Slag Remelting operation, as well as the results of the electrical impedance tomography, which is a technique to measure electrical quantities such as capacitance and impedance at ultra-high speed in multiple dimensions and visualize the concentration distribution in a multiphase flow field using an image reconstruction algorithm, to a suspension melted at a high temperature.

*Keywords: high temperature melts, AC field, electrical conductivity, electrical capacitance, impedance tomography*

# Thermodynamics analysis of slag-metal reactions in steel refining considering interactions of tramp elements for green steelmaking

**Hideki Ono**[1], Kengo Kato[2]

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## Abstract

Increasing the utilization of steel scrap is strongly required for reducing $CO_2$ emission in iron- and steel-making processes. In steel scrap recycling, the content of tramp elements in steel (such as copper and tin), which are difficult to be removed in steel refining, inevitably increases. Accordingly, it is essential to understand the thermodynamic characteristics relevant to the accumulation of tramp elements in molten steel. Due to the thermodynamic interactions, the tramp elements affect the activity of the other alloying elements in molten steel. To produce high-quality steel from steel scraps, the behavior of alloying elements should be precisely controlled. Therefore, the thermodynamic data of the interaction between tramp elements and alloying elements are needed. In this work, interaction coefficients of alloying elements with Cu and Sn in molten iron and Fe-18mass%Cr alloy were measured at 1873 K by a chemical equilibration technique. Thermodynamic analysis on slag-metal reactions in steel refining, including tramp elements, was subsequently performed using the obtained thermodynamic data. Molten steel composition will vary with the contents of impurities originating in iron resources and conditions of temperature and oxygen potential. The effects of scrap ratio on molten metal and slag composition were thermodynamically analyzed, and the effects of temperature and oxygen potential were discussed.

*Keywords: tramp element, recycling, steel scrap, interaction coefficient, thermodynamics.*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 3

November 20

16:00-18:00

# Technical **Oral Session _ Session 3**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 3 (A3)** — **16:00 - 17:50, Nov. 20**

**Chair :** To be announced — Halla Hall A, 3F

16:00-16:30 **K-A** **[Keynote]**
Peter Hodgson (Deakin University, Australia)

16:30-16:50 **I-A1026** **[Invited] A Novel Hot Work Die Steel Breaking Through the Contradiction between Strength and Thermal Conductivity**
Hongliang Yi (Northeastern University, China)

16:50-17:05 **O-A0327** **The study of the damage mechanism of dual-phase steel using in-situ X-ray Computed Tomography (XCT)**
Abdulwahab Qarooni (University Of Tokyo, Japan)

17:05-17:20 **O-A0119** **Analysis of martensitic transformation of metastable austenitic stainless steel during electrochemical polishing**
JunYoung Chae (Seoul National University, Korea)

17:20-17:35 **O-A0273** **Multi-aspect Characterization of Low-temperature Tempering Behaviors in High-carbon Martensite**
Yongjie Zhang (Tohoku University, Japan)

17:35-17:50 **O-A0290** **Three-dimensional configuration of deformation in stainless steel assessed by high resolution digital image correlation and confocal microscopy**
Wujun Yin (The University of Tokyo, Japan)

# A Novel Hot Work Die Steel Breaking Through the Contradiction between Strength and Thermal Conductivity

**Hongliang Yi[1,2]**, Lianqian Liu[1,2], Dapeng Yang[1], Shu Zhou[2]

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## Abstract

Strengthening of metals always relies on defects in crystals which hinder the glide of dislocations, whist the defects inhibit the movement of electronics and phonons, and consequently deteriorate the thermal conductivity of metals. In this research, a novel hot work die steel was designed to break through the contradiction between strength and thermal conductivity by changing the strengthening phase from incoherent alloy carbides in conventional hot work die steels to nano-sized coherent Cu and NiAl intermetallics precipitates. In addition, metallic precipitates and intermetallics with metallic bonds have much larger thermal conductivity compared to carbides with covalent bonds. The mass production of the novel alloy has been manufactured successfully by vacuum casting a 5 tons ingot followed by electroslag remelting and forging. Nano-sized precipitates of Cu and NiAl by aging process lead to the hardness increased to HRC49 from HRC34 in as-forged condition. The hardened alloy exhibits 40 W/m·K of thermal conductivity and 338 J of non-notched impact toughness, compared to 23 W/m·K and 189 J in conventional H13 hot-working die steels at the same hardness. The commercial application of the high thermal conductive steel would bring disruptive innovation by improving both efficiency and life of dies for either die-casting of aluminium alloys or hot-stamping of sheet steels.

*Keywords:* Hot work die steel; Precipitation hardening; Coherent interface; Cu precipitates; NiAl precipitates; Thermal conductivity

# In-situ micro-void observation during Tensile Testing by X-Ray computed tomography

(X 線 CT による引張試験中のマイクロボイドその場観察)

37-226952 Abdulwahab Qarooni; Supervisor: Prof. Manabu Enoki, Takayuki Shiraiwa

## 1. Introduction

X-Ray computed tomography (XCT) is a non-destructive evaluation method that allows observation of material microstructure on the surface and subsurface at micro meter level. It is applicable to various types of materials such as metals, ceramics, polymers, etc. Through XCT a 2D and 3D visualization of the material can be constructed using an image processing software. The 2D visuals are internal slices of the material which are then reconstructed into a 3D visualization. Furthermore, due to the high magnification of XCT it is possible to observe porosity, micro-voids and inclusions on the microstructure.

By performing in-situ XCT with tensile testing it is possible to observe the microstructure along with micro-void nucleation and their growth. This can then be used to study the fracture behavior of specimens under tension. Seo et al. [1] carried out in-situ observation of void nucleation and growth using X-ray tomography in a commercial steel and was able to visualize and quantify the voids within. The purpose of the present work is to carry out in-situ XCT while performing tensile testing in order to observe void nucleation and growth.

The purpose of this research is to study the ductile fracture mechanisms in DP steel by XCT during in situ tensile testing in order to obtain a better understanding on the effect of stress triaxiality on the void nucleation and the ductile fracture mechanism.

## 2. Experimental

The materials used for this experiment are DP steels consisting of martensite and ferrite phases. They are produced from the same commercial low-carbon steel ferrite-pearlite hot-rolled steel. By changing the heat treatment conditions, three samples with different phase morphologies and crystal grain shapes were manufactured. Different shapes of the specimens will be made in order to analyze the stress triaxiality and the effect it will have on void nucleation and fracture strain. Fig. (1) shows the schematic diagram of the heat treatment and optical micrographs of the different phase steels. The three specimens were named DP800, DP900 and DP1000 in relation to their tensile strength as analyzed from previous studies on the same specimen.

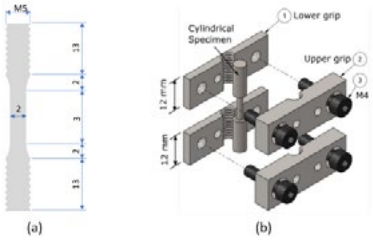



*Fig. 1:(a) Design of Duralumin. (b) Design of the specimen holder.*

The method of experimentation is as follows. The specimen is fixed onto the tensile machine and then into the XCT machine. The specimen's position is then set so that the region of interest (ROI) is in between the source and detector. The XCT parameters are then set and the specimen is subjected to uniaxial tensile test and then analyzed. The position of the specimen is readjusted to compensate for the change in position due to the elongation of the material. The results are then reconstructed into 2D and 3D images through an image processing software and analyzed in order to calculate the stress triaxiality, the microvoid nucleation and growth.

## 3. Results

## Reference

[1] D. Seo et al, ISIJ International, Vol. 55 (2015), No. 7, pp. 1474–1482
[2] F.H. Kim, S.P. Moylan, and E.J. Garboczi NISTIR 8234 (2019)

# Analysis of martensitic transformation of metastable austenitic stainless steel during electrochemical polishing

**Junyoung Chae**[1], Hojun Gwon[2], Chanwoo Jeong[3], Hyukjae Lee[4], Hyungjun Cho[5], Young-Kyun Kwon[6], Sung-Joon Kim[7], and Heung Nam Han[8†]

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## Abstract

It was newly observed that remarkable martensitic transformation occurs during electrochemical polishing (EP) in a 16Cr-5Ni metastable austenitic stainless steel. EBSD, XRD, and Ferritescope were used to identify whether martensitic transformation in a metastable austenitic stainless steel occurs. To elucidate the mechanism by which the EP induces the martensitic transformation, we calculated a charge build-up near the surface of stainless steel using COMSOL Multiphysics. Subsequently, we investigated the effects of the calculated charge build-up on the structural transformation during the EP by conducting first-principle calculations. The results revealed that considerable stress could be developed due to the charge build-up near the surface of the specimen, resulting in stress-induced martensitic transformation on the surface of the metastable austenitic stainless steel during EP. The kinetics of martensitic transformation during EP were investigated for stainless steel specimens with different surface roughness and austenite stability. It was found that specimens with higher surface roughness and lower austenite stability exhibited higher levels of martensitic transformation. The level of charge build-up at the specimen surface during EP was calculated using COMSOL Multiphysics for specimens with different surface roughness, and the stress effect was analyzed using first-principle calculations from preceding results. The results showed that specimens with higher surface roughness accumulated more charge build-up, inducing in a greater driving force for martensitic transformation. Additionally, the critical energy required for martensitic transformation was determined using Thermo-Calc for specimens with different austenite stability. The findings indicate that the martensitic transformation kinetics during EP can be explained in terms of austenite stability like stress-induced martensitic transformation.

*Keywords: Martensitic transformation, Electrochemical polishing, Electroplasticity, Multiphysics simulation, First-principle calculation.*

# Multi-aspect Characterization of Low-temperature Tempering Behaviors in High-carbon Martensite

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## Abstract

As-quenched martensite in carbon steels needs to be tempered to restore its ductility and toughness for practical applications. During tempering, a series of reactions relevant to carbon diffusion are known to occur sequentially, causing changes in microstructure in tempered martensite. In this study, multi-aspect characterization using various advanced characterization techniques was performed, with an aim to clarify the low-temperature tempering behaviors of high-carbon martensitic steels.

An Fe-0.8 mass%C binary alloy was mainly used in this study, and 4 ternary alloys with further 2 at% addition of Mn, Si, Cr or Al, were also investigated for comparison. All the alloys were water quenched after austenitization to obtain the as-quenched martensite as the starting microstructure. Tempering processes were performed either by continuous heating or isothermal holding under various conditions. Afterwards, the changes in physical properties of tempered martensite were analyzed via calorimetry, dilatometry, and resistometry, whereas the microstructural evolutions were characterized via transmission electron microscopy, in-situ neutron diffraction, and three-dimensional atom probe tomography.

The experimental results revealed the continuous occurrence of different tempering stages, including carbon clustering, precipitation of metastable iron carbide, decomposition of retained austenite, and precipitation of cementite. In addition, the tetragonality of martensite became continuously lowered due to the reduction in solute carbon content by tempering. Among all the investigated elements, the addition of Al was found to have the largest retardation effect on the tempering kinetics, which was attributed to its suppression effect on carbon clustering and carbide precipitation due to reduction in carbon diffusivity.

*Keywords: martensite, low-temperature tempering, multi-aspect characterization, carbon cluster, iron carbide.*

# Three-dimensional configuration of deformation in stainless steel assessed by high resolution digital image correlation and confocal microscopy

**Wujun Yin[1],** Fabien Briffod[1], Haoyu Hu[1], Takayuki Shiraiwa[1], Manabu Enoki[1]

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## Abstract

Austenitic stainless steels, which have superior corrosion resistance and good formability, are widely used in various important fields such as nuclear and medical in the past decades. An experimental study using high resolution digital image correlation (HR-DIC) had been carried out to investigate the slip activities at sub-grain scale, demonstrating that deformation occurred by the formation of slip bands well aligned with highly stressed slip systems. On the other hand, twinning was another important deformation mechanism in stainless steels. The evolution of a hierarchical microstructure through formation of twin bundles was reported. However, insufficient study of strain distribution of heterogeneous slip and twinning deformation as well as their interaction in austenitic stainless steel has prevented its further application. Therefore, this work aims to investigate the three-dimensional configuration of heterogeneous slip and twinning deformation in austenitic stainless steel through HR-DIC and laser scanning confocal microscopy (LSCM).

In this work, type 316 austenitic stainless steel was investigated by high resolution strain probing method including HR-DIC and LSCM. The microstructure of undeformed material and samples taken from uniaxial tensile tests were characterized by electron backscatter diffraction (EBSD) and LSCM. On the other hand, scanning electron microscope (SEM) were performed to obtain well-distributed patterns at each interval for HR-DIC analysis.

*Keywords: Austenitic stainless steel, three-dimension, HR-DIC, LSCM, strain localization.*

# Technical **Oral Session _ Session 3**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 3 (B3)** **16:00 -17:20, Nov. 20**

**Chair :** Kenta Yamanaka (Tohoku University), Myoung-Gyu Lee (Seoul National University) **301, 3F**

16:00-16:20 **I-B0437** **[Invited] Thermomechanical processing of interstitial high-entropy alloys**
Kenta Yamanaka (Tohoku University, Japan)

16:20-16:35 **O-B0135** **Real-time Flow Control of Liquid Steel based on Copper Plate Temperature by Fiber Optics Technology**
Hyun-Jin Cho (POSCO Technical Research Lab, Korea)

16:35-16:50 **O-B0643** **Vertical Bending Continuous Casting of Ferro-nickel Based Alloys for Photovoltaic Industry**
Pan Dong (Shanxi Taigang Stainless Steel Co., Ltd. (TISCO), China)

16:50-17:05 **O-B0729** **Development of sliding bearing using clad casting technology and improvement of mechanical properties of lining layers**
Soo-Yeon Lee (Pohang University of Science and Technology, Korea)

17:05-17:20 **O-B0518** **Preparation and simulation of high strength non-oriented silicon steel based on NiAl strengthening by strip casting**
Feng Fang (Northeastern University, China)

# Thermomechanical processing of interstitial high-entropy alloys

**Kenta Yamanaka**[1], Manami Mori[2], Kazuo Yoshida[3],
Yusuke Onuki[4], Shigeo Sato[5], Akihiko Chiba[6]

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## Abstract

Non-equimolar high-entropy alloys (HEAs) with low stacking fault energies exhibit transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP), demonstrating their great potential as a novel class of structural materials with excellent strength–ductility combinations. However, the yield strength of such alloys is often low for structural engineering applications and requires further improvement. In this study, we examined the synergetic effects of interstitial nitrogen addition and thermomechanical processing on the microstructure and mechanical behavior of metastable TRIP-assisted $Co_{20}Cr_{20}Fe_{34}Mn_{20}Ni_6$ HEA [1]. Hot compression tests and hot caliber rolling of the alloys with and without trace nitrogen addition (0.08 mass%) were performed at 700−1000 °C.

Both alloys consisted of single-phase face-centered cubic (fcc) microstructures in the annealed state, and nitrogen addition simultaneously improved the yield strength and tensile elongation. The results of hot compression tests revealed the occurrence of dynamic recrystallization and the formation of ultrafine-grained microstructures under optimal deformation conditions. Although phase decomposition during hot deformation was observed in both alloys, the precipitated phase changed with the nitrogen content. However, despite the relatively low applied strain, the N-doped alloy exhibited notable strengthening after hot-caliber rolling. Quantitative microstructural characterization via time-of-flight neutron diffraction revealed enhanced dislocation accumulation in the N-doped alloy compared to its N-free counterparts, suggesting that the interaction between nitrogen atoms and dislocations promoted dislocation strengthening upon hot caliber rolling.

[1] Z. Li et al., Acta Mater., 136 (2017) 262−270.

*Keywords: high-entropy alloys, interstitial nitrogen, thermomechanical processing, microstructure, neutron diffraction*

# Real-time Flow Control of Liquid Steel based on Copper Plate Temperature by Fiber Optics Technology

**Hyun-Jin Cho**[1]

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**Abstract**

In a continuous casting process, the flow state of molten steel inside a mold plays an important role for the quality of steel product. When the meniscus of molten steel is unstable, the liquid mold flux which covers the molten steel can be penetrated into molten steel and it is attached at the solidified shell. After rolling process, the surface defect is detected by entrapped mold flux. Especially, the instability of the flow state is further intensified by the occurrence of asymmetric flow when the SEN(Submerged Entry Nozzle) clogging is generated due to the accumulation of inclusions. Therefore, it is desirable to measure the liquid steel flow phenomenon inside the mold and control the flow to induce the stable condition. In the present study, the flow characteristics of liquid steel was investigated by using fiber optic technology. The temperatures of narrow-side copper plates were measured by inserting FBG(Fiber Bragg Grating) sensors and the flow behaviour of molten steel was studied through the temperature change. A specific location that can detect the meniscus flow was derived and a method for stabilizing the meniscus through real-time control of bias molten steel flow using EMS(Electro-Magnetic Stirrer) device was confirmed.

*Keywords: FBG sensor, Mold Flow Control, Asymmetric Flow*

# Development of sliding bearing using clad casting technology and improvement of mechanical properties of lining layers

**Soo-Yeon Lee[1]**, Jae Sang Lee[2], Yoon-Uk Heo[3], Dong Yeop Kim[4], Junil You[5], Eunsol An[6], Muha Kim[7], Kwanghee Lee[8], Dong Gyu Kim[9], Chang Hee Yim[10*]

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## Abstract

Aluminum alloy bearing is in the spotlight as a sliding bearing material with fatigue resistance, corrosion resistance, and wear resistance under high load, high temperature, high pressure, and high speed. In addition, when Sn is added to the Al alloy, the lubricating ability is improved, and thus high-quality products can be produced. However, Al-Sn alloys have a wide range of mushy zone and a large specific gravity difference, resulting in severe segregation during melting/casting. When manufacturing sliding bearings, the roll bonded cladding method is used to overcome this problem, secure the mechanical properties of the lining layer (Al-Sn-X alloy layer), and secure the bonding strength between the steel back and the Al-Sn-X alloy. However, the roll bonded cladding method has a limitation that cannot be applied to the manufacture of most other industrial bearings that use thick base metals applied to power generation systems, etc., except for engine bearings. Therefore, it is necessary to develop a clad casting technology to manufacture sliding bearings using thick base metal. Clad casting alone should also ensure the mechanical properties of the lining layer and the bonding strength between the steel rear and the Al-Sn-X alloy interface.

In this study, Al-Sn-X alloy design and mechanical property test were conducted as a way to secure the mechanical properties of the lining layer to develop sliding bearings using clad casting technology, and clad casting experiments were conducted to secure bonding strength between steel back and Al-Sn-X alloy interface.

*Keywords: Sliding bearing, Al-Sn-X alloy, Mechanical property, Bonding strength*

# Preparation and simulation of high strength non-oriented silicon steel based on NiAl strengthening by strip casting

**Feng Fang[1],** Diwen Hou[1], Yuanxiang Zhang[1], Yang Wang[1], Guo Yuan[1], Guodong Wang[1]

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## Abstract

In view of the demanding requirement of high-speed drive motor on non-oriented silicon steel, 0.35 mm high-strength non-oriented silicon steel based on NiAl phase strengthening was prepared by strip casting. The microstructure evolution and effect of NiAl precipitates on properties were analysed by OM, XRD, EBSD and TEM. Meanwhile, finite element simulation of mechanical and magnetic properties of motor core was conducted by ANSYS software. The results showed that the as-cast strip was mainly characterized with coarse columnar grains. The annealed sheet was consisted of medium α*, strong Goss and Cube and γ texture. High density of NiAl precipitates with an average size of 8~10 nm was obtained after peak aging. As a result, significant improvement in yield strength, as high as 889 MPa was obtained due to high anti-phase domain boundary of NiAl phase. Meanwhile, relatively good magnetic properties were obtained, with magnetic induction $B_{50}$ and iron loss $P_{1.0/400}$ of 1.62 T and 31.4 W/kg respectively. The simulation results showed that the maximum stress of silicon steel rotor was at the magnetic bridge. When the speed was greater than 12000 r/min, the maximum stress of the rotor was generally proportional to the speed by power 2.06. The experimental steel can be applied to permanent magnet synchronous motors with a maximum speed of 18000 r/min, together with excellent magnetic performance. Therefore, NiAl phase strengthening based on strip casting can provide a new approach for developing high strength non-oriented silicon steel for new energy vehicles.

*Keywords: non-oriented silicon steel; NiAl precipitates; mechanical properties; magnetic properties; strip casting*

# Technical **Oral Session _ Session 3**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 3 (C3)** **16:00 - 17:40, Nov. 20**

**Chair :** Youngsoo Yoo (Korea Institute of Materials Science) 201A, 2F

16:00-16:20 **I-C0827** **[Invited] Digital twin for control of dimensional accuracy of complex superalloy investment castings**
Da SHU (Shanghai Jiao Tong University, China)

16:20-16:40 **I-C** **[Invited] Fatigue Crack Growth Life Assessment in Ni-Based Superalloy Alloy 247LC at Elevated Temperatures**
Young Wha Ma (Doosan Enerbility Co., Ltd., Korea)

16:40-16:55 **O-C0080** **Research on the Secondary γ' Phase Precipitation Behavior of Single Crystal Superalloys by Aging Heat Treatment**
Xiaopeng Li (Harbin Engineering University, China)

16:55-17:10 **O-C0571** **Effect of Boron on the creep deformation of Inconel 617 Ni-based superalloys at 1273K**
DuHyun Kim (Korea Institute of Science and Technology, Korea)

17:10-17:25 **O-C0057** **Effect of secondary dendrite orientation on high temperature oxidation of a nickel-based single crystal superalloy**
Jiasheng Dong (Institute of Metal Research, Chinese Academy of Sciences, China)

17:25-17:40 **O-C0658** **Heat treatment design of Inconel 740H superalloy for microstructure stability and creep properties enhancement**
CheolHyeok Yang (Changwon National University, Korea)

# Digital twin for control of dimensional accuracy of complex superalloy investment castings

**Da Shu[1],** Bang Guan[2], Donghong Wang[3], Baode Sun[4]

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## Abstract

Investment casting is a primary process for manufacturing near-net-shape, complex geometry superalloy castings in aerospace sector. Various factors, including the shrinkage and deformation of wax pattern, yielding of the ceramic mold shell, and metal shrinkage during solidification, often result in casting defects in the form of unacceptable dimensional tolerances and distortion, which has been a significant challenge in the mass production of superalloy structural parts. In this presentation, we propose a digital twin framework for control of the dimensional accuracy of investment castings. Numerical simulations based on finite volume/finite element methods are employed to generate simulation data under different conditions, and then the physics based and data driven hybrid models are constructed through the POD-RBF (Proper Orthogonal Decomposition and Radial Basis Function) approach. This enables the development of reduced-order models for different stages in the investment casting process. Through the utilization of node matching algorithms and calculation method for displacement transfer between different process models, the cumulative displacement field of the final cast component is determined. As a result, the pre-design of the mold cavity can be achieved by counter-deforming all nodes with a comprehensive assessment of geometric displacement. Moreover, real-time control can be achieved by incorporating actual process parameters and collected data. By adjusting the mapping coefficients of the POD-RBF method, real-time displacement fields can be predicted and the process parameters can be optimized to minimize casting deformation. We demonstrate that the digital twin provides a powerful tool for online prediction and control of the complex investment casting process.

*Keywords: digital twin, investment casting, superalloys, dimensional accuracy, reduced-order models.*

# Research on the Secondary γ' Phase Precipitation Behavior of Single Crystal Superalloys by Aging Heat Treatment

**Xiaopeng Li[1],** Youshui Xie[2], Yao Hhuang[3], Chengzhi Zhao[4] , Hexin Zhang[5]

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## Abstract

The morphology and size of the γ' phase play a significant role in the fabrication of superalloy and the properties under severe conditions. The evolution of the size, morphology and distribution of γ' phase with holding time and solution temperature were discussed in detail and systematically in the present study. The γ' phase acquired after heat treatment exhibits a variety of morphologies, consisting of irregularly coarse primary γ' phase along the grain boundaries, cubeical secondary γ' phase homogeneously distributed on the matrix, and fine spherical tertiary γ' phase in γ matrix channel. With the increase of solution temperature from 1130°C to 1190°C, the size of secondary γ' phase gradually increases, while the size of tertiary γ' phase reaches the minimum value at 1160°C. At 1160°C, gradually the size of the secondary γ' phase increases as the solution time increases from 1.5h to 5.5h, while the size of the tertiary γ' phase reaches the minimum value 46.92nm at 3.5h holding time. In addition, the precipitation behavior of the tertiary γ' phase precipitated in the γ channel during aging is consistent with that of the γ' phase precipitated during solution cooling. This finding helps to understand the evolutionary behavior of the γ' phase in nickel-based superalloy during heat treatment and provides a fundamental theory for the optimization of the heat treatment of K444 alloy.

*Keywords: nickel-based single crystal superalloy; secondary γ' phase; nanoindentation; topography.*

# Effect of Boron on the creep deformation of Inconel 617 Ni-based superalloys at 1273K

**Du Hyun Kim**[1], Seok Su Sohn[2], Dong-Ik Kim[3], Jae-Hyeok Shim[4], Woo-Sang Jung[5], Jin-Yoo Suh[6]

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## Abstract

Minor addition of boron is known to increase creep resistance of Ni-based superalloys and its underlying mechanism has been a subject of number of research activities. In this study, we carried out creep experiment on Inconel 617 alloys with different boron contents at temperature of 923 and 973K which were measured by a set of conventional commercial creep testing machines and at 1273K by a custom-made equipment. At the high temperature as high as 1273K, creep rupture life turned out be longer for the alloys with higher boron content as in the case of conventional creep experiments done at 923 and 973K. With special attention on the fast kinetics at 1273K, creep deformation behaviour was additionally studied in different heating & loading conditions: creep rupture life of boron-containing alloy was enhanced for the case that the specimen was heated under load than the case where the load was applied after the specimen temperature reached to the target temperature, while the alloys without boron did not show such a difference. The observed behaviour suggests that the boron induced microstructural change during heating with the assistance of the applied load. Detailed microstructural characterization was carried out to discuss the origin of the enhanced creep resistance.

Topic : C, Structure material for high temperature

*Keywords: Creep, Inconel 617, Boron effect, Precipitates, Rupture behaviour*

# Effect of secondary dendrite orientation on high temperature oxidation of a nickel-based single crystal superalloy

Minghan Yu[1], **Jiasheng Dong[2]**, Li Wang[3], Jing Liu[4], Shiling Min[5], Yuping Ren[6], Hongxiao Li[7], Langhong Lou[8]

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## Abstract

High temperature oxidation is very important for advanced single crystal superalloys. Due to the anisotropy of single crystals, more and more attention has been paid to the effect of crystal orientation, especially, secondary dendrite orientation on mechanical properties. But little literature could be found in the open literature concerning the effect of secondary dendrite orientation on the oxidation of single crystal superalloys.

The effect of secondary dendrite orientation on oxidation behavior of a 3rd generation nickel-based single crystal superalloy at 1100 ºC was investigated in the present paper. The results showed that the mass gain of the samples with different secondary dendrite orientations increased in the order of [210], [110], and [100]. The [210] oriented samples show better high-temperature oxidation resistance due to the lowest mass gain. The secondary dendrite orientation affects the diffusion of various elements during oxidation and the stability of the oxidation products. Different spalling rate of oxidation products of the samples with different secondary dendrite orientations also cause different mass effects.

*Keywords: Oxidation; Single crystal superalloy; Secondary dendrite orientation; deformation; Spallation*

# Heat treatment design of Inconel 740H superalloy for microstructure stability and creep properties enhancement

**Cheol-Hyeok Yang**[1], Dong-Min Kim[2], Chiwon Kim[3], Hi-Won Jeong[4],Hyun-Uk Hong[5*]

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## Abstract

In this study, three heat treatment conditions selected from various heat treatment candidates for Inconel 740H, which are considered materials for A-USC steam turbines, were exposed to long-term thermal conditions at 750 ℃ up to 5,000 h. The stability and mechanical characteristics of heat-treated microstructure were examined, and the optimal heat treatment to maximize creep property was derived through the creep test (750 ℃/270 MPa). It was confirmed that the content of Cr was concentrated at the boundary of MC carbide without a specific orientation relationship at 750 °C/270 MPa creep, and this was the result of phase transformation by the reaction of MC + γ → $M_{23}C_6$ + γ'. Thus, MC carbide has high resistance to cracks because its temperature and stress during creep contribute to decomposition for phase transformation rather than initiation. Therefore, the higher the fraction of the MC carbide, the more advantageous it is to the creep property. In the case of superalloy developed within the component range of Inconel 740H, the fact that the fraction of MC carbides and M23C6 carbides decreased as the carbon and chromium contents decreased was confirmed through thermodynamic calculation. After the two types of heat treatment that we designed, the fraction and shape of grain boundary carbides were also different. This difference led to a result that continuous distribution and blocky type of carbide and γ' coarsened region which formed by creep stress and temperature induced optimizing the grain boundary deformation by dislocation gliding after the creep (750 ℃/270MPa).

*Keywords: Inconel 740H, Heat treatment, Creep properties, MC decomposition,* γ' coarsend retgion

# Technical **Oral Session _ Session 3**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 3 (D3)** **16:00 -18:05, Nov. 20**

**Chair :** Shinji Kumai (Tokyo Institute of Technology), Soong-Keun Hyun (Inha Unviersity) Samda Hall A, 3F

16:00-16:20 **I-D0409** **[Invited] A new Al-Si casting alloy with high elastic modulus**
Young-Hee Cho (Korea Institute of Materials Science, Korea)

16:20-16:35 **O-D0904** **Effect of Friction Stir Processesing On MIG Welded 5083 Alloy**
Jyoti Menghani (SVNIT SURAT, India)

16:35-16:50 **O-D0557** **A general framework for tension-compression asymmetry: theory and validation**
Yong Hou (Seoul National University, Korea)

16:50-17:05 **O-D0404** **Elucidation of wetting mechanism of aluminum brazing on silicon nitride by high-temperature wettability measurements**
Takumi Kusumoto (Yokohama National University, Japan)

17:05-17:20 **O-D0383** **Effect of initial microstructure on age-hardenability and thermal conductivity of Al-7Si-0.35Mg alloy**
Saif Kayani (Korea Institute of Materials Science, Korea)

17:20-17:35 **O-D0782** **The Effect of Solute Clusters on Dynamic Recovery of Al Alloys**
Yixin Wang (Monash University, Australia)

17:35-17:50 **O-D0193** **Effect of pre-deformation process on aging response and mechanical properties of Al-Zn-Mg-Cu alloys**
Cheon Hyunseok (Korea Institute of Materials Science, Korea)

17:50-18:05 **O-D1141** **Atomic-scale analysis of hydrogen embrittlement in high-strength Al alloys**
Huan Zhao (Xi'an Jiaotong University, China)

# A new Al-Si casting alloy with high elastic modulus

Yoon-Ho Lee[1,2], Jung-Moo Lee[1], Jae-il Jang[2], **Young-Hee Cho[1]**

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**Abstract**

Elastic modulus, a.k.a. Young's modulus is a measure of the stiffness or rigidity of a solid material, determined by the interatomic bonds. Pure aluminium has an elastic modulus in the reign of ~70 GPa and there have been extensive attempts to increase the modulus of aluminium alloys by introducing either ceramic particles or intermetallic phases having relatively higher elastic modulus than that of the aluminium matrix. We have recently developed new Al-Si based casting alloys with high elastic modulus in the range of 90-100 GPa and low density less than 3.0 g/cm$^3$, by alloy design and microstructural refinement approaches. Based on the preliminary study of alloying elements on the elastic modulus, microstructure and castability, we have selected new candidate alloys, hypereutectic Al-Si alloys with Ni additions, where large volume fractions (~40 vo.%) of hard primary Si and primary $Al_3Ni$ phases were present. However, coarse primary Si and primary $Al_3Ni$ formed upon solidification can interfere with the melt flow, reducing the castability and also were deleterious to elongation. By the assessments of the crystallographic misfit between a nucleant substrate and a nucleated solid, therefore, we discovered modifying elements to refine such coarse and brittle primary phases, particularly $Al_3Ni$. More importantly, along with the improved elastic modulus, an elongation of about 1% was achieved alongside advantageous yield strength of over 230MPa. Candidate application fields where the new high modulus aluminium casting alloys can be utilised are also suggested.

*Keywords: hypereutectic Al-Si alloy; casting; solidification; refinement; elastic modulus*

# Effect of Friction Stir Processesing on MIG Welded 5083 Alloy

**Jyoti Menghani**[1], Rohit Sharma[2]

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Friction stir processing (FSP) is emerging as a promising technique for making surface composites. FSP can improve surface properties such as abrasion resistance, hardness, strength, ductility, corrosion resistance, fatigue life and formability without affecting the bulk properties of the material. The welds are usually encountered with problems as porosity, distortions, loss of mechanical strength, stress concentration etc. In present investigation MIG welding is performed on 6 mm thick aluminium alloy 5083-H111 alloy at constant voltage (20 V)and varying welding current (105 A, 115 A, 125 A) and 15 lit/min argon shielding. FSP has been applied onto welds with varying rotational speed (1400 rpm, and 710 rpm) and transverse speed ( 28 mm/min and 40mm/min).Characterisation tests like hardness, tensile strength, vision measurements and microstructure study has been done for both, post processed and unprocessed weld. The results indicates improvement in hardness and tensile strength.

# A general framework for tension-compression asymmetry: theory and validation

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## Abstract

This study addresses the challenge in modelling complex plastic anisotropy-asymmetry of metallic materials, and presents a framework to resolve the problem by introducing a stress-triaxiality-dependent model parameter in the context of plasticity constitutive model. The proposed framework is general for applications under various stress states and flow rules with extended flexibility and accuracy. For example, the proposed modelling framework can reproduce the anisotropy of metals coupled with their tension-compression asymmetry in yield strength. The model can be applied to both 2D plane stress and 3D full stress states. Mathematical constraints are defined for the stress-triaxiality-dependent weighting factor using a fifth-order polynomial function under 2D loading. Case studies are conducted to validate the accuracy and effectiveness of the developed framework. As a result, the framework allows for different functions in tension and compression states, which enables to vary the accuracy in anisotropic modeling based on the data availability of tension and compression. Finally, proposed modelling framework demonstrates the evolutions of yield surfaces with plastic deformation for various materials covering from conventional metals to advanced lightweight sheet metals. As an example, the model can successfully describe the anisotropic-asymmetric plastic deformation of extruded Mg alloy under general 3D loading.

**Topic area**: Light Metals and Alloys

***Keywords***: *Plastic anisotropy; Tension-compression asymmetry; Stress triaxiality; Flow rule; Yield criterion*

# Elucidation of wetting mechanism of aluminum brazing on silicon nitride by high-temperature wettability measurements

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## Abstract

Bonding of aluminium heatsink and ceramic substrates with aluminum brazing is an important technology for functional components such as power semiconductors because heat generated at electric circuits has to be smoothly removed from the substrates. In general, however, thin aluminum oxide film formed during brazing lowers the wettability, and thus degrades the resultant joining strength between aluminium brazing and ceramic substrate. In this study, wetting mechanism between 2N-, 5N-purity aluminum or Al-12%Si alloy melt and silicon-nitride ($Si_3N_4$) was investigated by high-temperature wettability measurements and microstructural observation of the solidified aluminium brazing.

From the results of wettability measurements using a sessile drop method, it was found irrespective of the brazing compositions that oxide film disappears above 1300˚C, resulting in the improved wettability around θ=37-44˚ (Here, θ is wetting angle). Wettability was also improved at lower temperatures using an extrusion method, by which oxide film could be effectively removed by extruding aluminum brazing melt from a cylinder.

As a result of the diffusion of Si from $Si_3N_4$ to aluminum brazing melt, furthermore, aluminum-nitride was found to be formed as a reaction layer, together with the solidified aluminium brazing with higher amount of Si. Therefore, wetting mechanism between $Si_3N_4$ and aluminum brazing melt was supposed to involve both mass transfer and chemical reaction.

*Keywords: Wettability, Joining, Aluminum alloy, Silicon nitride ceramic, dissimilar material bonding*

# Effect of initial microstructure on age-hardenability and thermal conductivity of Al-7Si-0.35Mg alloy

**Saif Haider Kayani[1],** Kwangjun Euh[2], Jung-Moo Lee[3], Young-Hee Cho[4*]

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## Abstract

Age-hardenability and thermal conductivity are mutually exclusive in Al–Si–Mg alloys and are greatly affected by solute supersaturation and precipitation behavior. This research is a pioneering attempt to balance the hardness and thermal conductivity trade-offs of a casting product having various thicknesses by optimizing the processing conditions during casting, in particular, cooling rates during solidification. When using a step mold with cooling rates in the range of 2-50 K/s, the fast cooling rate, 50 K/s, exhibits high thermal conductivity in as-cast conditions owing to lower solute concentration and coarse pre-precipitation while retaining in the mold until solidification of other steps with slower cooling rates completes. The coarse pre-precipitation significantly reduces the age-hardenability of 50 K/s alloy during T5 heat treatment. Contrarily, the alloy solidified at a slow cooling rate (2 K/s) shows a stronger age-hardening behavior. The low thermal conductivity of as-cast 2 K/s alloy increases after age-hardening. It is observed that a small lattice misfit between precipitates and matrix in as-cast conditions induces large lattice distortion while lowering the alloy's thermal conductivity. After age-hardening, the lattice distortions are replaced by misfit dislocations at the precipitate-matrix interface owing to large misfits. Consequently, the thermal conductivity and hardness of alloys are improved. Finally, we demonstrate a minimum hardness-conductivity trade-off for alloy solidified at 2 K/s, yielding a colossal window to achieve property balance during the T5 treatment of Al–Si–Mg alloys.

*Keywords: Al–Si–Mg alloy, cooling rate, T5 treatment, precipitation hardening, thermal conductivity*

# The Effect of Solute Clusters on Dynamic Recovery of Al Alloys

**Yixin WANG[1],** Huan ZHAO[2], Xinren CHEN[2], Baptiste GAULT[2], Yves BRECHET[1], Christopher HUTCHINSON[1]

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**Abstract**

It is well known that solutes in solution can retard dynamic recovery in Al alloys. Mg is especially effective and this is used to good advantage in the highly formable 5xxx alloys. By this reasoning, it is expected that as solutes are removed from solid solutions, for example during a precipitation reaction, dynamic recovery becomes easier and this is often observed experimentally. However, this is not always the case and the arrangement of the solutes in the lattice can have important effects on the rate of dynamic recovery, especially in the case of early-stage decomposition of solid solutions following clustering reactions.

In this presentation, we describe the strain hardening behaviour of age hardenable Al-alloys as a function of precipitation state. We compare the as-quenched supersaturated solid solutions, with naturally aged, underaged and cyclic strengthened states under conditions where obstacle shearing dominates. We demonstrate that some alloys show that dynamic recovery first becomes more difficult as the yield strength increases, then, after passing through a minimum in dynamic recovery rate, dynamic recovery becomes easier as the yield strength continues to increase. We propose a model to link the macroscopic dynamic recovery behaviour to the underlying mechanisms of plasticity in relation to the distribution of solutes, clusters and precipitates in the studied alloys.

*Keywords: Al alloys; Dynamic recovery; Small-angle X-ray scattering; Atom probe tomography*

# Effect of pre-deformation process on aging response and mechanical properties of Al-Zn-Mg-Cu alloys

**Hyun-seok Cheon**[1], Su-hyeon Kim[21], Je In Lee[32]

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## Abstract

Aluminum alloys, due to their lightness and high strengths have been used in the transportation industries. 7000 series (Al-Zn-Mg) aluminum alloys have good mechanical properties, which can be further enhanced by changing various processing conditions in heat treatment and plastic deformation. In this study, the effect of pre-deformation before aging treatment on the mechanical properties was investigated using our newly developed Al-Zn-Mg-Cu alloys with high Zn content. The alloys with different Zn contents were cast, homogenized, hot-rolled, solution-treated, cold-rolled (pre-deformed) and artificially aged. Various rolling reductions were applied before the aging step to create structural differences, and we examined the effect of pre-deformation on mechanical properties after aging. Hardness and tensile tests were conducted to measure the mechanical properties, and SEM-EDS, EBSD, DSC, and TEM were used to analyze microstructural changes. The peak aging time was determined for each alloy from the hardness test results, and the alloys with higher Zn content had higher strengths at the peak aging conditions. The strengths increased with increasing the rolling reduction before aging, and decreased again when the reduction was higher than a certain amount. We discussed the role of dislocations formed during pre-deformation in the formation of GP zone or nucleation of precipitations to determine the strengths of the alloys.

*Keywords: Al-Zn-Mg-Cu alloys, pre-deformation, aging, strength, $MgZn_2$-$\eta$ precipitation*

# Atomic-scale analysis of hydrogen embrittlement in high-strength Al alloys

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**Abstract:**

Environmentally assisted embrittlement of high-strength Al alloys hinders their wide applications. The important role of hydrogen (H) associated with the H "embrittlement" mechanism occurs. However, the challenge of assessing the precise trapping sites of H makes the mechanisms remain ambiguous. We used atom probe tomography to investigate H associated with specific microstructural features in a high-strength 7xxx Al alloy. We successfully achieved visualization and assessment of H at second-phases and grain boundaries, with the enrichment of one order of magnitude higher as opposed to the Al matrix. We used these observations to guide atomistic ab initio calculations, which show that the co-segregation of alloying elements and H favours grain boundary decohesion, and the strong partitioning of H into the second-phase particles removes solute H from the matrix, hence preventing H embrittlement. Our insights further advance the mechanistic understanding of H-assisted embrittlement in Al alloys, emphasizing the role of H traps in minimizing cracking and guiding new alloy design.

Keywords: Hydrogen embrittlement, 7xxx Al alloy, Mechanical properties, Atom probe tomography, Ab-initio calculations

# Technical **Oral Session _ Session 3**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 3 (E3)** — **16:00 -17:50, Nov. 20**

**Chair :** Naoki TAKATA (Nagoya University) — Halla Hall B, 3F

16:00-16:30 **K-E0720** **[Keynote] Recent advances on powder development and evaluation for additive manufacturing**
Naoyuki NOMURA (Tohoku University, Japan)

16:30-16:50 **I-E1097** **[Invited] Alloy Design of High Temperature γ/γ' Ni-base Superalloy for 3D Printability**
Bhaskar Majumdar (New Mexico Tech., USA)

16:50-17:05 **O-E0863** **A high-temperature titanium alloy suitable for additive manufacturing**
Zhihao Zhu (Dalian University of Technology, China)

17:05-17:20 **O-E0737** **Microstructure and Mechanical Properties of Titanium Based Oxide Dispersion Strengthened Alloy Produced via Directed Energy Deposition**
Uijun Ko (Hanbat National University, Korea)

17:20-17:35 **O-E0476** **On the Hydrogen Embrittlement Resistance of Additively Manufactured Alloy 625 under Cathodic Protection Conditions**
Alex Kovacs (Curtin University, Australia)

17:35-17:50 **O-E1179** **Novel approach to manufacture powders with tailored chemical composition for Additive Manufacturing**
Bartosz Kalicki (Warsaw University of Technology, Poland)

# Recent advances on powder development and evaluation for additive manufacturing

**Naoyuki Nomura[1],** Weiwei Zhou[2], Zhenxing Zhou[3]

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## Abstract

The production and development of pure metal and alloy powders based on conventional powder metallurgy technology is expanding with the development of additive manufacturing (AM) technology. In particular, in the production of powders for AM, the characteristics of the powder shape according to the powder production process have been clarified, chemical composition and particle size control and have been implemented, and users are now in a situation where they can select powders according to application and cost. Studies on the evaluation and improvement of powder flowability and are still underway, although the current situation is that powder flowability should be ensured. The authors carried out discrete element method (DEM) simulations and recoating experiments for comparison. It has been shown that powder adhesion is responsible for flowability and is an important factor in controlling the density of the powder bed. In addition, the development of new alloys and composite powders for AM applications has been conducted intensively in recent years, but the large volume of powder production required for AM applications makes it difficult to speed up the development process. The development of composite powders, which cannot be produced using conventional technology, requires consideration of powder flowability in addition to homogeneity of composition. The authors also developed composite powder fabrication processes using hetero-aggregation method and freeze-dry pulsated orifice ejection method (FD-POEM) with considering the issues. In this presentation, the recent studies investigated by the authors will be introduced.

*Keywords: additive manufacturing, flowability, composite powder, flowability, freeze-dry pulsated orifice ejection method*

## | I-E1097 |

High temperature γ/γ' Ni-base superalloys have been difficult to fabricate microcrack-free using additive manufacturing (AM). Their high γ' volume-fraction (typically > 60 vol.%) and associated strength, along with poor weldability have been cited as possible reasons. Our research is focused on understanding the cracking mechanisms and making small alloy modifications to eliminate such solidification cracks. We have used CALPHAD and non-equilibrium Scheil model along with existing theories of solidification to understand the basis of cracking, and coupled that with our observation of microstructural defects at high angle grain boundaries where microcracks are found to occur. These experimental data were obtained from laser line scans of arc melted buttons of CM247LC, a widely used high-temperature Ni-base alloy with high volume fraction of $L1_2$ γ' phase, along with buttons with minor alloy modifications aimed at mitigating cracks. This approach circumvents the high cost and delay in procuring powders of different chemistries until a final alloy selection stage. EDS, elemental spectra, and TEM/EELS results will be presented to highlight the microcracking location and microstructural segregation, while also drawing attention to differences from predictions using non-equilibrium solidification models. We will demonstrate that this approach has for the first time resulted in a composition that completely eliminates cracking during AM of this high temperature alloy class.

Keywords: Ni-base superalloy, additive manufacturing, gamma/gamma-prime, microcracking, 3-D printability

# A high-temperature titanium alloy suitable for additive manufacturing

**Zhihao Zhu**[1], Tianyu Liu[2], Qing Wang[3], Chuang Dong[4]

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## Abstract

High-temperature Ti alloys generally show poor additive manufacturing processibility. We here report a high-temperature alloy, Ti-6.8Al-6.8Zr-2.3V-2.1Mo-0.7Nb, suitable for laser additive manufacturing. This alloy is designed using the cluster formula approach: the composition of a solid solution is rooted in a structural unit covering a nearest-neighbor cluster plus a few next-neighbor glue atoms. Its composition formula consists of twelve α-Ti units, $\{[Al\text{-}Ti_{12}](AlTi_2)\}_{12}$, and five β-Ti ones, $\{[Al\text{-}Ti_{12}Zr_2](AlV_{1.2}Mo_{0.6}Nb_{0.2})\}_5$, which is modified from that of popular Ti-6Al-4V with enhanced β stability via Zr, Mo, Nb, and V co-alloying. The surface is quite shinny and the bulk is nearly pore-free. In the as-deposited state, it exhibits a bimodal basket-weave structure with quite high ultimate tensile strength (UTS) of 1348 MPa and yield strength (YS) of 1253 MPa, and a moderate elongation of 4.4%. At 600 ℃, its UTS of 657 MPa, YS of 578 MPa, and particularly elongation of 44.6% are better than those of wrought-state high-temperature Ti alloys. At 650 ℃, its UTS of 424 MPa and YS of 337 MPa still maintains a high level.

*Keywords: Ti alloys; cluster formula; laser additive manufacturing; microstructure; mechanical properties.*

# Microstructure and Mechanical Properties of Titanium Based Oxide Dispersion Strengthened Alloy Produced via Directed Energy Deposition

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## Abstract

This research was conducted as a preliminary research to verify the feasibility of Ti-based oxide dispersion strengthened (ODS) alloy. Pure-Ti powder was mixed with $Y_2O_3$ powder and then, mechanically alloyed at -150 ℃. Ti-based ODS powder was recrystallized by directed energy deposition. The microstructure consisted of elongated grains and Y excess fine particles. The oxide particle size was larger then that of typical Fe-based ODS steels. Tensile test showed that tensile ductility was around 25% while the strength is much higher than that of pure Ti. High-temperature hardness of the Ti-ODS alloy was also much higher than that of pure Ti at all temperatures whilst lower than that of Ti-6Al-4V. Dimple structure was well developed and no evidence of cleavage fracture surface was observed in the fracture surface of the tensile specimen.

*Keywords: Oxide dispersion strengthened, Titanium, Additive manufacturing, mechanical properties, Directed energy deposition*

# On the Hydrogen Embrittlement Resistance of Additively Manufactured Alloy 625 under Cathodic Protection Conditions

**Alex Kovacs[1],** Thaneshan Sapanathan[1], Mobin Salasi[1], Mariano Iannuzzi[1], Zakaria Quadir[2], Christopher Hutchinson[3]

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## Abstract

Nickel alloys, particularly UNS N06625 (Inconel 625), are commonly used in the oil and gas industry in environments unsuitable for conventional stainless steel. When used in subsea components, nickel-based alloys can be coupled with carbon and low alloy steels under cathodic protection, which can lead to the generation of atomic hydrogen at the surface. Atomic hydrogen can then diffuse into nickel alloy components and, under specific conditions, lead to hydrogen embrittlement, a significant concern for the industry. In this study, the hydrogen embrittlement (HE) resistance of Inconel 625 manufactured by Laser Powder Bed Fusion (LPBF)—also known as Selective Laser Melting (SLM)—is investigated and compared with the conventional wrought counterpart. The experiments were performed using the step-loading tensile test method based on the ASTM F1624-12 standard. The tensile samples were charged with hydrogen in 0.6M NaCl (unadjusted pH approximately 6.0) at a galvanostatic current of -50mA, equivalent to -1.4VAgACl. Samples were first pre-charged for 48 h before the in-situ Step Loading test. Charging continued during loading. Results indicated that SLM625 outperformed wrought Inconel 625 in both the grade 1 and grade 2 conditions, exhibiting an excellent HE resistance irrespective of printing direction.

*Keywords: Hydrogen Embrittlement, Inconel 625, Selective laser melting, Additive Manufacturing, Cathodic Protection*

# Novel approach to manufacture powders with tailored chemical composition for Additive Manufacturing

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## Abstract

The technology of ultrasonic atomization itself is quite old, but due to technological and material limitations available in the 1950s-80s, it has been almost completely supplanted by gas and plasma atomization technologies. Nevertheless, these commonly used methods, despite obtaining spherical powders of high purity and appropriate granulation, require the use of a large amount of material. In industrial settings, this is an advantage in high-volume production, but unit manufacturing processes dedicated to specific implementations, or prototyping currently carried out with 3D printing technologies, require much smaller amounts of powder, which is provided by ultrasonic atomizers. This technique also has another significant advantage and other methods of manufacturing alloy powders. A small amount of batch materials allows, under laboratory conditions, rapid validation of the chemical composition, phase structure and mechanical properties of newly designed alloys with specific, strictly dedicated performance properties.

*Keywords: additive manufacturing, metallic powders, atomization, ultrasonic atomizaiton, powder bed fusion*

# Technical **Oral Session _ Session 3**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 3 (F3)** **16:00 - 17:40, Nov. 20**

**Chair :** Seong Keun Kim (Korea Institute of Science and Technology) 202A, 2F

16:00-16:20 **I-F0178** **[Invited] Unassisted Solar water splitting via Organometal Halide Perovskite-Based dual Photoelectrodes**
Sanghan Lee (Gwangju Institute of Science and Technology, Korea)

16:20-16:40 **I-F0902** **[Invited] Enhanced surface reactivity by severe plastic deformation: application to the hydrogen and biomedical sectors**
Thierry Grosdidier (Université de Lorraine, France)

16:40-16:55 **O-F0906** **Modulating the structure and properties of NbMoTaW high-entropy thin films by interatomic interactions**
Xiao Wang (Dalian University of Technology, China)

16:55-17:10 **O-F0512** **Insights into effects of O-mediated sputtering toward improving Ag wetting on oxides**
Jungheum Yun (Korea Institute of Materials Science, Korea)

17:10-17:25 **O-F0908** **Resistivity behavior and magnetic properties of CoCrFeNi-based high-entropy thin films**
Xiaona Li (Dalian University of Technology, China)

# Unassisted Solar water splitting via Organometal Halide Perovskite-Based dual Photoelectrodes

**Sanghan Lee[1]**

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## Abstract

Photoelecrochemical (PEC) water splitting is most promising process which can produce green hydrogen. To achieve efficient and stable unassisted solar water splitting, development of organometal halide perovskite (OHP)-based photoelectrodes is highly desired due to the excellent optoelectronic characteristics. However, stable utilization of OHP-based photoelectrodes is significantly challenging because they are vulnerable to water molecules. In this talk, highly efficient and stable OHP-based photoelectrodes achieved by metal encapsulation method will be introduced. Furthermore, the OHP-based dual photoelectrodes for unassisted solar water splitting will be discussed. We successfully fabricated OHP-based PEC systems composed of highly efficient and stable OHP photocathodes and photoanodes. We believe that the OHP-based PEC system afford us opportunities to achieve the future practical application of OHP-based PEC systems for efficient and stable solar $H_2$ production.

*Keywords: Photoelectrochemical, Organometal halide perovskite, unassisted solar water splitting, green hydrogen*

# Enhanced surface reactivity by severe plastic deformation: application to the hydrogen and biomedical sectors

**Thierry Grosdidier**[1,2], Marc Novelli[1,2], Laurent Weiss[1,2]

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## Abstract

After a short recall of various techniques using shots to induce Surface Severe Plastic Deformation (SSPD) and a brief survey of the advantages of having a gradient structure for mechanical properties, the effects of the processing parameters and temperature of deformation on the surface roughness and subsurface microstructure modifications are illustrated with a particular emphasis on the surface mechanical attrition treatment (SMAT) and ultrasonic shot peening (USP) techniques deriving from the traditional pre-strain shot peening.

In addition to affect mechanical properties such as fatigue, recent developments take advantages of the "reactivity" of these modified surfaces in the fields of corrosion and "duplex" surface treatments. In these cases, in addition to induce grain refinement and dislocations, the importance of controlling some potential surface contamination is stressed.

Finally, the contribution will illustrate some new research studies with potential applications for challenges: (i) in the hydrogen sector for its solid-state storage and the protection of mechanical infrastructures as well as (ii) for bio-medical applications.

*Keywords: Surface, Severe Plastic Deformation (SPD), Fatigue, Hydrogen storage, Bio-compatibility.*

# Modulating the structure and properties of NbMoTaW high-entropy thin films by interatomic interactions

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## Abstract

High entropy alloys (HEAs) are solid solutions with the specific local structure. The addition of different elements can lead to change in the local structure, which ultimately affects the properties. However, the observation of the local structure is very difficult and limited. Therefore, a simplified local structure model is proposed, which will play a key role in the property analysis of HEAs. We choose the weak enthalpy interaction element V and the strong interaction element O to modulate the local structure of NbMoTaW films: The addition of V does not change the body-centered-cubic (BCC) structure of the films, but it can make the hardness and modulus show a small increase and then slowly decrease trend. The films have relatively low electrical resistivities and excellent high temperature stability. The addition of O leads to a gradual transition of the films from O-containing BCC solid solution to the amorphous oxides. The hardness and modulus initially increase and then decrease. Additionally, this transition causes a shift in the film's electrical conduction mechanism from metallic to amorphous semiconductor-type. Utilizing the cluster-plus-glue-atom model, the local structure of the films can be effectively analyzed, enabling the prediction of performance changes. This provides an effective method for the design of functional compositions in high entropy alloys.

*Keywords: Cluster-plus-glue-atom; High entropy alloys; Local structure; Interatomic interactions*

# Insights into effects of O-mediated sputtering toward improving Ag wetting on oxides

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## Abstract

A defect-free, highly crystalline, ultrathin Ag layer demonstrates remarkable characteristics in terms of minimizing electrical and optical losses within the given geometry. These properties make it an ideal choice for transparent electrodes in optoelectronic devices, where both high electrical conductance and optical transmittance are required. Nevertheless, achieving a completely continuous, two-dimensional (2D) layered structure at extremely small thickness remains a formidable challenge where the utilization of nonnoble metallic elements like Cr, Cu, Ti, and Ni is discouraged due to their inferior optoelectrical properties.

In this study, we present a novel approach involving the O-mediated growth of ultrathin 2D Ag layers on oxide substrates. By manipulating the cohesion of Ag and the adhesion between Ag and oxide, we successfully achieve a substantial decrease in free energy. Experimental and numerical evidence demonstrate that the improvement in Ag wetting can be attained by simultaneously decreasing the surface and interface free energy. This O-induced free energy decrease is primarily attributed to the migration and segregation of incorporating atomic O along the outer boundaries of evolving Ag structures. The results also confirm that the spontaneous dissipation of atomic O from Ag lattices leads to the complete reduction of thermodynamically unstable Ag suboxides. This dynamic sequence of O interstitials leads to a significant enhancement of the electrical and optical properties of Ag films in oxide/Ag/oxide configurations. By employing atomic O-mediated Ag growth and subsequent spontaneous reduction of Ag oxides, it becomes possible to implement highly efficient Ag film electrodes with exceptionally low optoelectrical losses.

*Keywords: ultrathin Ag film, transparent electrode, atomic O incorporation*

# Resistivity behavior and magnetic properties of CoCrFeNi-based high-entropy thin films

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## Abstract

The CoCrFeNi-based high entropy alloy thin films (HEATFs) have excellent application prospects due to their outstanding electrical properties and magnetic potential. Therefore, it is very important to study the influencing factors of film properties. By adding different elements, we explore the fundamental cause of the change of resistivity behavior and magnetic properties. The addition of Al allows for a wide range adjustment of resistivity while maintaining the ultralow temperature coefficient of resistance (TCR), thus exhibiting excellent high-temperature stability. After native oxidation of CoCrFeNi film, the core-shell structure is naturally formed, with ferromagnetic Fe, Co, and Ni as the core, and Cr oxide as the shell. The unique core-shell structure improves the soft magnetic properties and resistivity of the films, which provides a new idea for the design of high entropy soft magnetic thin films. The addition of Al alters the core-shell structure and changes the shell layer to an Al oxide, which affects the magnetic properties. Overall, the CoCrFeNi-based HEATFs have stable TCR, which are suitable for high-temperature applications. Moreover, by modulating the compositions, the core-shell structure under native oxidation can also be changed, which can achieve a wide range of modulation of the properties to suit different applications.

*Keywords: High-entropy thin films; Native oxidation; Resistivity–temperature behavior; Soft magnetic*

# Technical **Oral Session _ Session 3**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 3 (G3)** **16:00 - 18:05, Nov. 20**

**Chair :** Young-Bum Chun (Korea Atomic Energy Research Institute) 303A, 3F

16:00-16:30 **K-G0854** **[Keynote] Temperature-dependent synergistic evolution mechanism of rhenium and irradiation defects in tungsten**
Hong-Bo Zhou (Beihang University, China)

16:30-16:50 **I-G0814** **[Invited] Rectifying and antiport of cations by metal-organic framework–based nanochannel membrane for osmotic energy harvesting**
Jun Lu (Monash University, Australia)

16:50-17:05 **O-G0974** **Effects of Crystallite Size on the Water Intercalation and Heat Storage Properties of Layered Manganese Dioxide**
Hiroki Yoshisako (Tohoku University, Japan)

17:05-17:20 **O-G0356** **Preparation of Porous Iron Whisker and its Evaluation for Cyclic Oxidation/Reduction Property by H2-H2O**
Anri Suzumura (Tohoku University, Japan)

17:20-17:35 **O-G0230** **Effect of Mg grain size on formation of MgH2**
Wataru Kitano (Kansai University, Japan)

17:35-17:50 **O-G0917** **Mechanisms of hydrogen transportation and hydrogen-induced damage in tungsten as an armour material for fusion devices**
Long Cheng (Beihang University, China)

17:50-18:05 **O-G0862** **Heterointerface engineering of NiFe/Y2O3 hybrids for high-efficient alkaline water splitting**
Zhen Xin Hui (Jilin University, China)

# Temperature-dependent synergistic evolution mechanism of rhenium and irradiation defects in tungsten

**Hong-Bo Zhou**, Yu-Hao Li, Guang-Hong Lu

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## Abstract

Tungsten (W) is one of the most promising candidates for plasma facing materials (PFMs) in future fusion reactors. Rhenium (Re) is not only the typical alloying elements but also the main productions of transmutation in W-PFMs. More importantly, Re will aggregate and precipitate in W under high energy radiation, which substantially enhance the radiation hardening and embrittlement, leading to the great concerns for the life-limiting of W-PFMs. So far, the formation mechanism of Re-rich clusters in W remains to be fully elucidated.

We have systemically investigated the synergistic evolution of Re and irradiation defects in W under different temperatures and irradiation doses using object Kinetic Monte Carlo method. Our results revealed the underlying mechanism for the transition of Re effect on W from beneficial to harmful during the Re-defects evolution with the increasing of irradiation dose, in which temperature always plays a critical role. On the one hand, Re will significantly promote the defect annihilation at low irradiation dose and high temperature, thereby effectively reducing their sizes and number densities. This is due to the formation of stable Re-SIAs complexes that can be eliminated by the mobile vacancy-type defects, whereas the transition of the migration pattern of SIAs only plays a weak role on the defect recombination in W-Re system. On the other hand, with the increasing of irradiation dose, Re will aggregate to form Re-rich clusters or even precipitates. Interestingly, the formation mechanism of Re-rich clusters is also dependent on temperature. At low temperatures, the interstitial-mediated mechanism plays a crucial role in the Re-rich cluster formation, while at high temperatures, both SIA-type and vacancy-type defects will act as the transport carriers of Re to promote their clustering. Accordingly, the critical conditions for the transition of Re from beneficial to harmful and the formation of Re-rich clusters at different temperatures and irradiation doses are given with the help of the phase diagram. Our work presents the temperature dependence of the synergy of Re and irradiation defects in W in fusion-relevant environment, which provides a good reference for the development of radiation-resistant materials and the prediction of W performance in fusion reactors.

*Keywords: synergistic evolution, irradiation defects, defects recombination, rhenium-rich clusters, tungsten*

# Rectifying and antiport of cations by metal-organic framework–based nanochannel membrane for osmotic energy harvesting

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## Abstract

Bioinspired control of ion transport at the sub-nanoscale has become a major focus in the fields of nanofluidics and membrane separation. It is fundamentally important to achieve rectifying ion-specific transport in artificial ion channels, but it remains a challenge. To the best of our knowledge, it remains a challenge to achieve unidirectional transport of metal ions and proton with rectifying direction opposite each other in the same artificial ion channel while having high ion conductance. Since the individual rectifying metal ion conduction or proton conduction is important for many applications such as in energy harvesting and storage and membrane separation, the realization of the dual ion rectifying property would represent a significant step forward for the design of more efficient devices in these areas. Here we report a novel metal-organic framework nanochannel (MOF NC) membrane to achieve unidirectional ultrafast counter-directional transport of alkaline metal ions and proton. This unprecedented ion-specific rectifying transport behaviour is attributed to two distinct mechanisms for metal ions and proton, elucidated by theoretical simulations. Notably, the MOF NC exhibits ultrafast proton conduction stemming from ultrahigh proton mobility and low energy barrier in MOF sub-nanochannels. As a proof of concept, this MOF NC membrane exhibits promising osmotic energy harvesting performance. This work expects to inspire further research into multifunctional biomimetic ion channels for advanced nanofluidics, biomimetics, and separation applications.

*Keywords: Nanofluidics, Biomimetic ion channel, Osmotic energy harvesting, Rectifying ion transport, Metal-organic frameworks,*

# Effects of Crystallite Size on the Water Intercalation and Heat Storage Properties of Layered Manganese Dioxide

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## Abstract

Low-grade waste heat (100−200°C) accounts for more than 60% of the industrial waste heat. Recovery and reuse of low-grade waste heat are required to realize sustainable energy use. Heat storage technology, which can release stored heat on demand, is considered as one of the promising solutions for harvesting the low-grade waste heat. Heat storage materials can be categorized into several groups according to heat storage mechanisms: sensible-heat, phase-change, physisorption, chemisorption, and chemical-reaction types. Although intensive studies on each type of heat storage materials have been made, no material has so far been reported that simultaneously exhibits the properties required for a good heat storage material, such as high energy density, reversibility, rate of heat absorption/desorption and so on.

Through studies on the phase stability of various manganese dioxide polymorphs [1], our research group recently found that layered manganese dioxide (birnessite, δ-$K_{0.33}MnO_2$) can absorb heat below 160°C via dehydration of crystal water. Moreover, we found that heat absorption/release of δ-$K_{0.33}MnO_2$ can reversibly occur via water (de)intercalation mechanism where water molecules are released/absorbed from/into the interlayer [2]. This water intercalation mechanism is categorized into the physisorption-type heat storage. Because of its high energy density (>1,000 MJ/m$^3$), reversibility, fast reaction rate, and abundance of the material, the layered manganese dioxide is expected to be a promising high-performance heat storage material. In order to further develop this material as a heat storage material, we have investigated the heat storage properties of δ-$K_xMnO_2$ ($x$ ~ 0.33) with different crystallite sizes synthesized by several synthesis methods.

[1] T. Hatakeyama, N. L. Okamoto and T. Ichitsubo: *J. Solid State Chem.*, **305**, 122683 (2022).
[2] T. Hatakeyama, N. L. Okamoto, S. Otake, H. Sato, H. Y. Li and T. Ichitsubo: *Nat. Commun.*, **13**, 1452 (2022).

*Keywords: low-grade waste heat, heat storage materials, physisorption, water intercalation, crystallite size*

# Preparation of Porous Iron Whisker and its Evaluation for Cyclic Oxidation/Reduction Property by $H_2$-$H_2O$

**Anri Suzumura**[1], Takumi Kobayashi[2], Daisuke Maruoka[3], Taichi Murakami[4], Eiki Kasai[5], Naoki Yamamoto[6]

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## Abstract

Cyclic redox reaction of iron powder with water vapor and hydrogen has been proposed as one of a safety hydrogen storage method. The idea is that magnetite is first reduced to metallic iron using hydrogen, and oxidation of magnetite by water vapor generates hydrogen when necessary. This method is more economical way to apply to hydrogen storage and release system since iron can be obtained easily and is enough in resources. However, the problem is the decrease in $H_2$ production capacity and production rate due to the decrease in specific surface area caused by the sintering of iron powder as the number of redox cycles increases. In a previous study, we reported that the iron whisker powder prepared by the carbothermic reduction using iron oxide and biomass char has a higher $H_2$ production rate during $H_2O$ oxidation than commercial iron powder samples. In this study, the optimization of iron whisker morphology by adding Sc, Ti, V, Y, Zr, Nb, and Hf oxides and the effect of these additives on the repeatability of the redox reaction were evaluated. The results indicated that various shapes of iron whisker were obtained depending on the oxide additions. In particular, the iron whisker prepared by adding vanadium and hafnium oxides showed a high aspect ratio. Furthermore, the iron whisker prepared with vanadium oxide indicated to maintain repeatability performance approximately 10% higher than the sample without addition.

*Keywords: Hydrogen Storage, Iron Whisker, Iron Powder, Cyclic Redox Reaction, Sustainable Technologies*

# Effect of Mg grain size on formation of $MgH_2$

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## Abstract

In this study, the rate of $MgH_2$ formation was shown to be constant per Mg grain boundary length. As Kondo et al reports, during Mg hydrogenation process, $MgH_2$ formed not only on the surface(sur) but also internal phase(int). The $MgH_2$(int) hasn't any interface with the $MgH_2$(sur), and internal defects, such as grain boundary, residual strain and intermetallic phases in Mg are responsible for the formation and growth of $MgH_2$(int). Assuming that Mg grain boundaries directly influence the formation of $MgH_2$(int), the rate of $MgH_2$(int) formation could be estimated to be constant per grain boundary length. In order to verify this assumption, different grain sizes of Mg were prepared(52-156 μm), hydrogenation was conducted on these samples and the formation density, particle size and particle morphology of the $MgH_2$(int) were evaluated. Hydrogenation time versus $MgH_2$(int) formation density was extrapolated and the rate of $MgH_2$(int) formation per Mg grain boundary length was found to be 7-9 x $10^{-3}$ $mm^{-1}$ $h^{-1}$ at 673 K and under 4.0 $MPaH_2$. For calculating the equation, $MgH_2$(int) with low circularity and coarse grain size were excluded because they were assumed to be aggregates resulting from the initial $MgH_2$(int) generating residual strain in the surrounding Mg. This result indicates that Mg grain boundaries influence the formation of $MgH_2$ but not its growth.

*Keywords: $MgH_2$, grain boundary, formation rate, number density, grain morphology*

# Mechanisms of hydrogen transportation and hydrogen-induced damage in tungsten as an armour material for fusion devices

**Long Cheng[1]**, Yue Yuan[2], Guang-Hong Lu[3]

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## Abstract

The success of commercial fusion energy relies on not only sustaining a steady-state burning fusion plasma, but also reasonable component lifetimes. Tungsten as an armour material forms the boundary in between fusion plasma and the reactor vessel, and experiences a harsh environment including irradiation by high flux hydrogen plasma, high heat flux and 14 MeV neutron. Hydrogen-tungsten interaction could deteriorate surface integrity by blistering and raise radioactive risk by building up tritium inventory. It is therefore important to understand mechanisms of hydrogen transportation and hydrogen-induced blistering, which could contribute to novel material designs for increasing material lifetime in terms of hydrogen-induced damage.

High flux deuterium plasma irradiation experiments with high fluences at temperature of 500 K were performed using recrystallized tungsten in the linear plasma device to reproduce edge plasma conditions as in a fusion device. Transmission electron microscope studies demonstrate details of microstructures of blisters and the <001> edge dislocation nucleation mechanism of blistering is revealed. Deuterium diffusion and trapping in tungsten were investigated using nuclear reaction analysis and thermal desorption spectroscopy. The measured deuterium retention is proportional to the square root of the fluence, implying a plausible inference that deuterium diffusion length follows the same relationship. However, detailed rate theory modelling of plasma irradiation and thermal desorption clearly shows the diffusion length is proportional to the 0.32 power of the fluence, inferring important roles of defect production rate and surface morphology on deuterium transportation. The proposed mechanisms provided a new insight into hydrogen-tungsten interaction for fusion application.

*Keywords: deuterium, tungsten, blister, thermal desorption, fusion*

# Heterointerface engineering of $NiFe/Y_2O_3$ hybrids for high-efficient alkaline water splitting

**Zhen Xin Hui**[1], Chun Cheng Yang [2]

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## Abstract

The construction of high-performance and cost-effective electrocatalysts towards hydrogen/oxygen evolution reaction (HER/OER) is critical for industrialization of hydrogen energy by water electrolysis, which still remains challenging. In this work, a highly active and durable $NiFe/Y_2O_3$ hybrids electrocatalyst with abundant metal-rare earth oxide heterointerfaces is rationally constructed. Experimental results and theoretical calculations reveal that $Y_2O_3$ can assist $H_2O$ dissociation at the $NiFe/Y_2O_3$ heterointerfaces, and the charge redistribution induced by interfacial Ni/Fe-O-Y bonds can regulate the energy band structure to optimize the adsorption of intermediates. As a result, $NiFe/Y_2O_3$ exhibits low overpotential of 27 mV at 10 mA $cm^{-2}$, low Tafel slope of 52 mV $dec^{-1}$, and robust stability of 400 h at 200 mA $cm^{-2}$ for HER. The $NiFe/Y_2O_3$ also shows outstanding performance toward overall water splitting with a low cell voltage of 1.64 V at 100 mA $cm^{-2}$. It is anticipated that this work would enlighten the application of rare earth oxides in the catalytic field of water electrolysis.

*Keywords: Heterointerface engineering, $NiFe/Y_2O_3$, rare earth oxides, water splitting, DFT simulations*

# Technical **Oral Session _ Session 3**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 3 (H3)** **16:00 - 18:10, Nov. 20**

**Chair :** Sanghoon Kim (University of Ulsan) 303B, 3F

16:00-16:30 **K-H1077** **[Keynote] Current induced dynamics of magnetic skyrmion and its application**
Joonyeon Chang (Korea Institute of Science and Technology, Korea)

16:30-16:50 **I-H1084** **[Invited] Spintronic device based on van der Waals Materials**
Guoqiang Yu (Chinese Academy of Sciences, China)

16:50-17:10 **I-H1171** **[Invited] Giant Field-Like Torque from Bulk Rashba Effect in the Artificial Superlattices**
Sanghoon Kim (University of Ulsan, Korea)

17:10-17:25 **O-H1010** **Atomic-scale Understanding of Periodic Modulation in Heusler Alloy Ni-Mn-Ti**
Die Liu (Xi'an Jiaotong University, China)

17:25-17:40 **O-H0991** **The study of topological skyrmions in Kagome magnets**
Ying Zhang (Institute of Physics, Chinese Academy of Science, China)

17:40-17:55 **O-H0931** **Impression of magnetism, critical behaviour and magnetocaloric effect in FeNi alloy**
MOHIT KUMAR SHARMA (Changwon National University, Korea)

17:55-18:10 **O-H1080** **Oxide Insulated High-performance Soft Magnetic Composites**
Xuefeng Zhang (Hangzhou Dianzi University, China)

# Current induced dynamics of magnetic skyrmion and its application

**Joonyeon Chang**[1], Kyung Mee Song[2], Seonghoon Woo[1,2]

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Most magnetic materials show collinear magnetic ordering due to the large exchange interaction between neighbouring magnetic moments. If provided the Dzyaloshinskii-Moriya interaction (DMI) is strong enough to overcome the exchange interaction, magnetic spins tend to align in a non-collinear manner with fixed homochirality. In any structures where the broken inversion symmetry leads to sufficiently large DMI, non-trivial small cylindrical swirling spin structures, called magnetic skyrmions can be energetically stable. Magnetic skyrmions are topologically protected spin textures that have nanoscale dimensions and can be manipulated by an electric current. These properties make the structures potential information carriers in data storage, processing and transmission devices.

The room temperature stabilization of magnetic skyrmions and their current pulse-induced displacement on nano-tracks has been reported in magnetic heterostructures. The deterministic writng and deleting of a single isolated magnetic skyrmion is required for fully functional skyrmionic devices.

In order to utilize skyrmion for any electronic devices, we have studied current driven dynamics of skyrmions and inhibition of the skyrmion Hall effect which is detrimental to application. We have shown that the current-induced manipulation of skyrmions at room temperature can be used to store information as well as to mimic the potentiation and depression behaviours of biological synapses. In particular, the accumulation and dissipation of magnetic skyrmions in ferrimagnetic multilayers can be controlled with electrical pulses. In this talk, I will briefly introduce current induced dynamics of skyrmions and discuss about future application of skyrmions in terms of non-volatile memory and synapse devices for neuromorphic computing.

**Keywords:** skyrmion, DMI, skyrmion Hall effect, synapse device,

# Spintronic device based on van der Waals Materials

Guoqiang Yu

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## Abstract

Spintronic devices constructed based on electron spin properties are expected to be applied in information storage and processing. In order to achieve high-performance spintronic devices, people need to develop efficient methods for manipulating magnetic moments and reading magnetic moment states electrically. 2D van der Waals materials, due to their numerous advantages, such as diverse types, ability to overcome lattice mismatch and build high-quality heterojunctions, diverse crystal structures and symmetries, strong spin-orbit coupling, and adjustable conductivity, provide an ideal material platform for the research and development of spin electronic devices. This report will outline the research progress of the author and collaborators on the electrical manipulation and reading of magnetic moments in heterojunctions based on two-dimensional van der Waals materials.

[1] *Nature Communications* 14, 382414 (2023)

[2] *Chinese Physics Letters Express Letter* 40, 058501 (2023)

[3] *Advanced Materials* 32, 2000513 (2020)

[4] *Science Advances* 5, eaaw8904 (2019)

*Keywords: spintronics, 2D, van der Waals material, ferromagnet*

# Giant Field-Like Torque from Bulk Rashba Effect in the Artificial Superlattices

**Sanghoon Kim**

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Spin-orbit interaction plays a crucial role for magnetization control via spin current in heterostructures composed of non-magnetic and ferromagnetic materials. Among the elements in the periodic table, such as Pt and W, which have large atomic numbers as the 5d metals, there have been reports of spin current that enables magnetization control. Additionally, efforts to achieve switching current densities below $10^{10}$ A/m$^2$ for efficient magnetization control have been made in low-dimensional materials such as topological insulators like $Bi_2Se_3$ and van der Waals materials like $WTe_2$. An important point is that the developed heterostructures must be suitable for unit structures in spin-orbit torque (SOT) magnetic random access memory (MRAM), and compatible with CMOS processes for practical applications. From this point of view, topological insulators and van der Waals materials may not be suitable for MRAM development.

In this study, we demonstrate that bulk Rashba-type band splitting is formed in an asymmetric artificial superlattice of W/Co/Pt, fabricated using atomic-level deposition techniques [1]. Due to the sizable Rashba effect, the superlattice generates spin current over 300% more efficient than Pt. Our theoretical reveal that such large bulk Rashba effect originates from orbital asymmetry induced by a W atomic layer, which is also confirmed by the x-ray magnetic circular dichroism study. Our result suggest that artificial structure without symmetry can be promising system for spin current generation.

*Keywords: Spin-orbit interaction, Rashba effect, artificial superlattice, spin current*

[1] W. S. Ham, et al. Adv Sci. **10**, 2206800 (2023).

# Atomic-scale Understanding of Periodic Modulation in Heusler Alloy Ni-Mn-Ti

**Die Liu**[1], Yao Liu [2], and Tianyu Ma[3*]

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## Abstract

Periodically modulated martensites, such as 5M, 6M, 7M and 4O, have been frequently observed in Ni-Mn-based Heusler alloys. Associated with these modulated martensitic transformations, appealing properties, such as large magnetic field-induced strain, giant magnetocaloric, and elastocaloric effects, have been reported, offering enormous potential for advanced industrial applications. However, understanding of the formation of modulated structures has prompted much controversy between atomic shuffling (or periodic distortion) and adaptive phase (or nano-twinning, assembly of blocks with fixed lattice parameters) concepts. The main difficulty lies in the capturing of atomic re-arrangement process for martensitic transformation with fast kinetics. In this work, the atomic re-arrangement process from B2 austenite to 4O (4-layer modulated orthorhombic) martensite in a $Ni_{50}Mn_{32}Ti_{18}$ Heusler alloy with giant elastocaloric effect was investigated through in-situ cooling TEM and HR-TEM. The results showed that this alloy undergoes a two-step martensitic transformation, from B2 to 3O and further to 4O, upon cooling. During the modulation period change from 3O to 4O, the lattice parameters are also adjusted, together with the gradual formation and dissociation of $\{110\}<1\bar{1}0>_{B2}$-type stacking faults. The 3O and 4O phases have distinct tetragonality in the assembling blocks if following the adaptive phase concept, which supports that atomic shuffling may account for the formation of modulated martensites. Consequently, this study may deepen the understanding of modulated phase transformation in an important class of functional alloys.

*Keywords: Heusler Alloy; Modulated martensites; Electron microscopy.*

**We wish to make oral presentation at Symposium H (Electronic and Magnetic Materials) in PRICM11.**

| O-H0991 |

# The study of topological skyrmions in Kagome magnets

**Ying Zhang [1], Zhuolin Li [2], and Baogen Shen[3]**

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## Abstract

The unique geometric frustrated Kagome lattices, electronic correlation effect, topological quantum state and other new features of Kagome magnet is of great significance for the development of quantum technology. The recent discovery of a topological Chern phase in the spin–orbit-coupled Kagome lattice $TbMn_6Sn_6$ has attracted considerable interest, highlighting the contribution of momentum space Berry curvature and Chern gap on the electronic transport properties. The intrinsic real space magnetic texture is crucial for understanding the electronic properties and further exploring the unique quantum behavior but remains elusive. In this talk, by using lorentz transmission electron microscopy, the stabilization of topological magnetic skyrmions is directly demonstrated near room temperature, where the spins experience full spin reorientation transition between the a- and c-axes. An effective spin Hamiltonian based on the Ginzburg–Landau theory is constructed and micromagnetic simulation is performed to clarify the critical role of Ruderman– Kittel–Kasuya–Yosida interaction on the stabilization of skyrmion lattice. The manipulation of topological skyrmion has fundamentally advanced the understanding in condensed matter physics and potential applications in next generation quantum information technology.

*Keywords: Kagome lattice, quantum magnet $TbMn_6Sn_6$, Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction, topological Hall conductivity, topological skyrmion*

# Impression of magnetism, critical behaviour and magnetocaloric effect in FeNi alloy

**Mohit K. Sharma**[1], Akshay Kumar[2], Kavita Kumari[3], Naveen Yadav[4], Haw-In Lee[5], Seok-Hwan Huh[6], Bon-Heun Koo[7*]

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## Abstract

In the present study, we have investigated the detailed structural, magnetic and magnetocaloric properties of Fe50Ni50 alloy. The polycrystalline FeNi alloy has been synthesized by the ball milling method, followed by annealing and quenching. This sample is further characterized by x-ray diffraction, magnetic and magnetocaloric measurements. Rietveld analysis of structural results indicates the cubic crystallographic phase with Fm-3m space group. Magnetization results confirmed the soft ferromagnetic nature and obtained Curie temperature (TC) around 762 K. Effective magnetic anisotropy and saturation magnetization (MS) are obtained from magnetic isotherms. MS follow the modified Bloch law, and the results reinstate the ferromagnetic nature of the alloy. Arrott plot study confirmed the second-order nature of this alloy. Critical exponent was also further determined by using a modified Arrott plot, Kouvel-Fisher law and critical isotherms method. The results indicated the existence of ferromagnetic ordering along with short-range interaction and inhomogeneous magnetic state. Magnetocaloric parameters in the form of magnetic entropy change (–ΔSM) and relative cooling power (RCP) are also studied. Both parameters have shown significant values (ΔSM ~ 2.3 J/kg-K, RCP~ 230 J/kg at 30 kOe applied field) in the vicinity region and follow the power law behaviour with the magnetic field. For this alloy, a universal master curve from ΔSM data is also constructed, again confirming the second-order nature of magnetic phase transition.

**Keywords:** FeNi alloy, Magnetism, Arrott plot, Critical behaviour, Magnetocaloric effect.

Submitting Topic: H (Electronic and Magnetic Materials)

# Oxide Insulated High-performance Soft Magnetic Composites

Xuefeng Zhang

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**ABSTRACT**

Soft magnetic composites (SMCs) consisting of insulated metallic magnetic particles are critical materials in modern electronics. However, traditional SMCs are faced with low permeability and low mechanical strength due to the vulnerable and non-magnetic insulation layer. Here, we succeed in fabricating FeSiAl based SMCs by confined interfacial reaction between FeSiAl matrix and two oxides ($TiO_2$, $MoO_3$). $TiO_2$ can progressively release O atoms, leads to the formation of homogeneous and lattice-matched $Al_2O_3$ layer and brings about effective electrical insulation of FeSiAl particles. Meanwhile, itself becomes ferromagnetic with deficient oxygen, resulting in high permeability. $MoO_3$ has low melting temperature, and the redox reaction between FeSiAl and $MoO_3$ melt greatly reduces the interfacial energy, facilitates fully wetting of FeSiAl particles by $MoO_3$ melt, and promotes the liquid-phase sintering and insulation of metallic magnetic particles in one step. Our work provides alternative concepts for designing new SMCs, and will promote the development of high-performance power electronics.

**Keywords:** Soft magnetic composites; confined solid-state reaction; liquid-phase sintering; permeability; power loss

# Technical **Oral Session _ Session 3**

## **Symposium I :** Biomaterials and Soft Materials and their Application

**Biomaterials and Soft Materials and their Application 3 (I3)** **16:00 -17:45, Nov. 20**

**Chair :** Masaya YAMAMOTO (Tohoku University), Akio KISHIDA (Tokyo Medical and Dental University) **400, 4F**

16:00-16:30 **K-I0214** **[Keynote] Biomaterials-based delivery of signaling molecules and cells for tissue regeneration**
Heungsoo SHIN (Hanyang University, Korea)

16:30-16:45 **O-I0435** **Matrix-bound nanovesicles (MBVs) extracted from various decellularized tissues for neuroregenerative effects.**
Mako Kobayashi (Tohoku University, Japan)

16:45-17:00 **O-I0663** **Radially Expanding Mucoadhesive Gelapins for Intestinal Retentive Applications**
Durva Naik (Carnegie Mellon University, USA)

17:00-17:15 **O-I0574** **Variation of Ni ion release behavior of a pulsed-anodized NiTi alloy surface by a voltage setting**
Ryota Kawakami (Kitami Institute of Technology, Japan)

17:15-17:30 **O-I0440** **Engineered biomaterials for control of bone matrix organization via osteocytes-osteoblasts communication**
Tadaaki Matsuzaka (Osaka University, Japan)

17:30-17:45 **O-I0644** **Development of novel titanium surface with both long-term antibacterial property and hard-tissue compatibility by two-step micro arc oxidation process**
Yusuke TSUTSUMI (National Institute for Materials Science, Japan)

# Biomaterials-based delivery of signaling molecules and cells for tissue regeneration

**Heungsoo Shin**

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**Abstract**

For several decades, tissue engineering has garnered significant attention for its potential to replace or repair damaged or diseased tissues and organs by harnessing the body's own natural repair mechanisms. While cell-based therapies have shown promise, challenges remain in delivering cells to the site of injury, and promoting their survival and integration into host tissue. Biomaterials may offer a viable solution by creating a supportive microenvironment for cell growth, differentiation, and integration. Specifically, biocompatible materials can be tailored to present signaling molecules, such as growth factors, cytokines and small molecules, in a controlled manner to promote tissue regeneration. Various techniques, including physical and chemical immobilization, have been developed for this purpose. In parallel, multi-cellular spheroids, which mimic tissue and organ structure, have been extensively studied as a 3D assembly module for engineering organ-like architectures. However, spheroids present issues including hypoxia caused by intense cell-cell interactions, a lack of precise control over cell functionality, and limited ability to replicate the spatial organization of native 3D tissue structures. To address these challenges, biomaterials can also be utilized to create spheroids with enhanced properties and to support them to recapitulate complex tissue architecture. This presentation details our approaches to using biomaterials for surface-mediated delivery of signaling molecules and their integration with spheroids for musculoskeletal tissue regeneration.

*Keywords: tissue engineering, stem cells, spheroids, 3D biofabrication, growth factor delivery*

# Matrix-bound nanovesicles (MBVs) extracted from various decellularized tissues for neuroregenerative effects.

**Mako Kobayashi [1, 2]**, Jun Negishi [2, 3], Yoshihide Hashimoto [2], Masaya Yamamoto [1], Yoshihiro Sasaki [4], Kazunari Akiyoshi [4], Tsuyoshi Kimura [2], Akio Kishida [2]

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## Abstract

Matrix-bound nanovesicles (MBVs), which are tightly bound to the extracellular matrix, have recently attracted attention as one of the bioactive components of decellularized tissues. MBVs do not express exosome markers, suggesting that they are a new type of extracellular vesicles. In our previous studies, MBVs were extracted from high hydrostatic pressured (HHP)-decellularized tissues developed in our laboratory. They induced vascular endothelial cell's proliferation. Based on this study, we focused on nerve regeneration, which is essential for tissue reconstruction, and examined the neuroregenerative effects of MBVs derived from HHP-decellularized tissues. Nanosized and membranous vesicles which contain miRNA and small RNA can be extracted from decellularized tissues. Neurite outgrowth was observed when various decellularized derived-MBVs were added to PC12 cells and mouse dorsal root ganglion. Thereafter, the MBVs were mixed with fibrin gel and applied to the injured site in a rat sciatic nerve injury model; by week 6, rats treated with gel mixed with the abovementioned MBVs showed a statistically higher sciatic function index (SFI) than that of injured rats. Also, axons were wrapped by Schwann cells and elongated in the direction of the fibers, similar to the uninjured group. Taken together, these results indicate that the MBVs can induce nerve regeneration and functional recovery. Further, this study provides useful insights into the development of highly functional materials by compositing MBVs.

*Keywords: Decellularized tissue, matrix-bound nanovesicle, nerve regeneration*

# Radially Expanding Mucoadhesive Gelapins for Intestinal Retentive Applications

**Durva A. Naik**[1], Xiaozili Huang[2], Nihar Trivedi[3], Christopher J. Bettinger[4]

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## Abstract

Improving patient compliance to medication and enabling real-time gut health monitoring can be achieved through long-term retention of drug-delivery implants or medical devices in the small intestine. Previous techniques such as mechano and chemo-adhesion, however, present certain drawbacks. Mechano-adhesion, which involve intestinal tissue piercing systems, carries the risk of bacterial infection with long-term use while chemoadhesion techniques encounter the challenge of rapid eradication due to constant mucus turnover. Here, we introduce gelapin biodegradable hydrogels prepared by crosslinking gelatin with genipin – a natural protein crosslinker, which facilitate synergistic mucoadhesion with the intestinal tissue by creating interpenetrating networks with its mucosa, thus overcoming mucus turnover-related elimination. Gelapins are further cast into self-expanding mucoadhesive cylinders with optimized swelling capacity and chemo-adhesion for oral delivery. Gelapin formulations with 25% crosslinked sites demonstrate a maximum normal adhesion of nearly 50 μJ/mm² and a swelling capacity of approximately 1050% within 48 hours. Adhesion gradually increases over time, showing a sixfold increase within 4 hours which is attributed to genipin elution from the porous gelapins which facilitates crosslinking of mucin glycoproteins. Mucoadhesive cylinders exhibit a radial expansion of 50% within one hour, resulting in a final diameter of ~2.3 cm which is comparable to the diameter of the small intestine. This study therefore validates the use of gelapins as compliant chemo-adhesive material to develop long-term intestinal retentive devices.

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TOPIC AREA: Biomaterials and Soft Materials and their Application

*Keywords: Mucoadhesion, Hydrogels, Biodegradable, Intestinal-retention, Radial-expansion*

# Variation of Ni ion release behavior of a pulsed-anodized NiTi alloy surface by a voltage setting

**Ryota Kawakami**[1], Kasumi Tate[2], Yuya Matsui[3], Akihiro Tsuruta[4], Naofumi Ohtsu[5]

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## Abstract

The Ni ion release from NiTi alloys into the human body causes cytotoxicity, becoming a significant concern when used as biomaterials such as cardiovascular stents and implants. Our group found out that anodization in a nitric acid electrolyte using pulsed-waveform voltage formed a Ni-free $TiO_2$ layer on the alloy, thereby suppressing the Ni-ion release. In this study, we investigated the effect of the lower voltage in the pulsed-waveform on Ni ion release behavior aiming to the further suppression effect, for enhancing the suppression further. expecting further suppression. The rectangular pulsed-waveform voltage with the upper voltage of 3.5 V and pulse width of 100 ms was used for anodization, wherein, the lower voltage was decreased from 3.5 to 0 V stepwisely. The anodized alloy surfaces were then characterized using SEM and XPS. Additionally, the amount of Ni ion released from the alloys into a physiological solution was evaluated. The thickness of the anodized layer was increased with decreasing the lower voltage in the pulsed-waveform; besides, the Ni concentration in the anodized layer was decreased concomitantly. Electrochemical analysis showed that the corrosion resistance of the anodized alloys ware comparable, while Ni ion release decreased with decreasing the lower voltage. Based on the above, we inferred that the Ni ion release from the pulse anodized surface is predominated by Ni concentration in the surface layer, not from the corrosion protectivity. In conclusion, the lower-voltage setting in pulsed anodization is a significant factor that relates to the suppression of Ni ion release.

*Keywords: NiTi alloy, pulsed anodization, Ni-free $TiO_2$, Ni ion release.*

# Engineered biomaterials for control of bone matrix organization via osteocytes-osteoblasts communication

**Tadaaki Matsuzaka**, Aira Matsugaki, Takayoshi Nakano

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## Abstract

Alteration of collagen/apatite bone matrix microstructure in response to external loading stimuli is a crucial factor in determining the functional adaptation of bone tissue. While the mechanotransduction in bones is largely governed by osteocyte function, the precise mechanisms linking mechanical stimuli and bone matrix microstructural organization are not yet fully understood. Here, we propose a novel co-culture device that allows for simultaneous control of mechanical stimuli to osteocytes and the response of osteoblasts alignment which determine the subsequent bone matrix organization.

The stress-responsive mature osteocytes were isolated using a fluorescent-activated cell sorter (FACS). Osteoblasts isolated from newborn mice were seeded onto the collagen scaffolds with molecular orientation. The obtained two kinds of cells were cultured via nanopore membrane which enables intercellular communication via soluble factors. The dynamics of fluid flow stimuli to osteocytes were regulated using Particle Image Velocimetry (PIV). Gene expression changes in osteocytes were analyzed by RNA sequencing to identify the molecules determining bone matrix organization in response to mechanical stimuli.

Mechanical stimuli with oscillatory flow modulated osteocyte regulation of osteoblast arrangement. Specifically, the release of cytokines from osteocytes in response to oscillatory stimuli promoted the degree of preferred alignment of osteoblasts along the scaffold arrangement. Moreover, we successfully determined the dominant factor Prostaglandin E2 (PGE2) that controls the oriented microstructure of the bone matrix under mechanical stimuli. PGE2 controlled the cytoskeletal regulation of osteoblasts and further determined the microstructure organization of bone matrix secreted by the aligned osteoblasts. This is the first report of PGE2 role as a bone functional regulator through structuring bone matrix anisotropic texture.

*Keywords: Osteocyte, Mechanosensing, Functional adaptation, Osteoblast arrangement, Bone matrix microstructure*

# Development of novel titanium surface with both long-term antibacterial property and hard-tissue compatibility by two-step micro arc oxidation process

**Yusuke Tsutsumi**[1], Harumi Tsutsumi[2], Masaya Shimabukuro[2], Peng Chen[2], Masakazu Kawashita[2], Hideki Katayama[1], Takao Hanawa[2]

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## Abstract

A customized micro-arc oxidation (MAO) treatment technique was developed to obtain antibacterial properties with no toxicity on Ti surfaces. A two-step MAO treatment was used to fabricate a specimen containing both Ag and Zn in its surface oxide layer, and the optimal incorporation conditions were determined. Surface characterization by EDS was performed followed by the antibacterial properties against Escherichia coli (*E. coli*) and Staphylococcus aureus (*S. aureus*) and osteogenic cell compatibility evaluations. In addition, metal ion release tests were performed to evaluate the contents of Ag and Zn and the ion release behavior in order to simulate practical usage. MAO-treated specimens prepared using proper concentrations of Ag and Zn (0.5Ag-5Zn:0.5 mM $AgNO_3$ and 5.0 mM ZnCl, respectively) exhibited excellent antibacterial properties against *E. coli* and *S. aureus* and no toxicity to MC3T3-E1 in antibacterial and cytotoxic evaluations, respectively. The antibacterial property of 0.5Ag-5Zn against S. aureus was sustained even after two months of immersion in physiological saline, simulating the *in vivo* environment.

*Keywords: Antibacterial properties; Micro-arc oxidation; Silver; Titanium; Zinc.*

# Technical **Oral Session _ Session 3**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 3 (J3)** **16:00 -18:10, Nov. 20**

**Chair :** Eita TOCHIGI (The University of Tokyo) 201B, 2F

16:00-16:30 **K-J0873** **[Keynote] Strain localisation in engineering alloys – quantifying discrete shear to improve understanding of plasticity and crack initiation**
Michael Preuss (Monash University, Australia)

16:30-16:50 **I-J0225** **[Invited] Recent Advances of Synchrotron 4D X-ray Tomography with Millisecond-Order Temporal Resolution**
Wataru YASHIRO (Tohoku University, Japan)

16:50-17:10 **I-J0728** **[Invited] Tracking hydrogen-induced microstructural evolution in materials using in situ scanning electron microscope techniques**
Jin Woo Kim (Korea Institute of Science and Technology, Korea)

17:10-17:25 **O-J0432** **Characterization of Ni nano-particles by laboratory high energy Ultra-Small Angle X-ray Scattering (USAXS)**
Masato Ohnuma (Hokkaido University, Japan)

17:25-17:40 **O-J0412** **In-Situ Study of Liquid-Liquid Phase Separation Behavior in Cu-Fe Alloys by Synchrotron X-ray Imaging**
Daehoon Jeong (Pohang University Of Science And Technology, Korea)

17:40-17:55 **O-J0183** **In-Situ SEM Observation Combined with DIC Strain Analysis for Understanding Deformation and Cracking in Metal Coatings**
Dasom Kim (Nagoya University, Japan)

17:55-18:10 **O-J0517** **Study of crack propagation, dislocation movement and deformation twin evolution in Al-Sc alloy during in-situ TEM tension**
Zhongwei Chen (Northwestern Polytechnical University, China)

# Strain localisation in engineering alloys – quantifying discrete shear to improve understanding of plasticity and crack initiation

**Michael Preuss**[1, 2], Doncheng Hu[2], Yukun Xu[2], Conghui Liu[2], David Lunt[2], Laure Bourgeois[1], Joao Quinta da Fonseca[2]

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**Abstract**

Plastic deformation in alloys is typically highly localised creating stress concentrations at the microstructural scale that can lead to premature failure. The discrete shear develops into heterogeneous strain patterns, which might depend on microstructural parameters, and which will affect strain hardening and crack initiation.

Recent advancements in imaging nano-patterned mechanical test samples in a SEM for high resolution digital image correlation (HRDIC) has opened new possibilities of understanding the impact of alloy chemistry and microstructures on the degree of strain localisation that develops during monotonic or cyclic loading. I will present examples of utilising HRDIC to quantify the effect of alloy chemistry and microstructures on the degree of strain localisation that raises interesting questions related to for example solid solution strengthening. I will also provide an outlook of the direction of travel with the development of fully integrated in-situ SEM systems enabling the automation of the complex imaging/loading procedures.

*Keywords: strain localisation, digital image correlation, crack initiation*

# Recent Advances of Synchrotron 4D X-ray Tomography with Millisecond-Order Temporal Resolution

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## Abstract

There are increasing demands for visualization of internal structures with high spatio-temporal resolution in various fields of materials and life sciences. Synchrotron X-ray tomography can meet these demands. We successfully realized millisecond-order temporal-resolution synchrotron radiation X-ray tomography for rotating samples, using white synchrotron radiation from a bending magnet at SPring-8, and achieved even 4D (3D + time) X-ray tomography with 5 μm spatial resolution and 10 ms temporal resolution [1,2]. However, it is difficult to precisely control the environment around the sample at high rotational speeds of tens of thousands of rpm or more. In addition, 4D tomography of liquids and living organisms is impossible due to the centrifugal forces associated with high-speed rotation. To solve these problems, it was desired to realize high-speed 4D X-ray tomography without sample rotation. Recently, we developed a new multi-beam X-ray optical system for high-speed 4D X-ray tomography without sample rotation [3]. Using this system, we demonstrated that a 3D tomographic image can be reconstructed from 32 projection images covering ±70 degrees even with an exposure time of 1 ms. It is also possible to realize element-selective 4D X-ray tomography. Our approach is expected to have various applications in the fields of materials science and life science.

References
[1] Appl. Phys. Express 10 (2017) 052501; Jpn. J. Appl. Phys. 56 (2017) 112503; Appl. Phys. Express 11 (2018) 122501.
[2] J. Synchrotron Rad. 28 (2021) 322; https://www.youtube.com/watch?v=4D2RLSmY0kg
[3] Optica 7 (2020) 515.

*Keywords: X-rays, Imaging, Tomography, Synchrotron, Millisecond*

# Tracking hydrogen-induced microstructural evolution in materials using in situ scanning electron microscope techniques

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## Abstract

Understanding hydrogen (H) transport within a material microstructure and consequent microstructural changes can aid in designing novel energy materials for H infrastructure such as efficient solid-state H storage materials and H-embrittlement resistant materials for structural applications. However, it is challenging to observe and analyze H effects due to the complexity of its interactions with various defects and constituents in material microstructures, as well as its high diffusivity in materials. To overcome these difficulties, we developed novel in situ H-charging techniques that are compatible with scanning electron microscopy (SEM) and high-energy X-ray diffraction. The first generation of the in situ H-charging setups employs an electrochemical cell to insert H into a disc-type bulk specimen, which allows investigating the effect of H-ingress in a relatively short time scale but only at room temperature. The second generation of techniques currently being developed utilizes a microscale heater and H gas environment, which would enable to study H-induced microstructural evolution in a pressurized H environment at an elevated temperature up to 1073K. These SEM-compatible and versatile techniques enable real-time imaging, crystallographic analysis, and micromechanical analysis during H-ingress into a specimen. Through several case studies on titanium-based H-storage alloys and structural alloys, we demonstrate how in situ SEM techniques can be used to address the complex challenge of H-induced effects on material microstructures.

*Keywords: in situ SEM, hydrogen embrittlement, hydrogen storage, hydride formation*

# Characterization of Ni nano-particles by laboratory high energy Ultra-Small Angle X-ray Scattering (USAXS)

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**Abstract**

Evaluating dispersion of nano-particles is important in electronics industries. However, due to the high absorption of light, some of the particles such as Ni, cannot be characterized by common light scattering. It is also difficult to characterize it using laboratory SAXS with regular Cu-Kα line. Therefore, purpose of this study was to establish a technique to measure Ni powder, paste, and sheet in the same way using high energy laboratory Ultra-Small Angle X-ray Scattering device(USAXS).

Ni nano-particles with powder, paste, and sheets were placed between two cover glasses with a thickness of 0.15mm. An O-ring with a thickness of 0.25 mm was placed between them. All samples were tested using the Bonse-Hart type USAXS system with Mo target in transmission mode to observe changes in scattering angle and intensity.

A shoulder-like scattering profile was obtained in both paste and sheet states as well as in powder state, allowing for evaluation of Ni particle size. Position of appearance of shoulder-like scattering depends on the size of raw particles. After desmearing the profiles, we analysed the size distribution by fitting. All of the measured profiles also shows the scattering from aggregation structure. They are more found in paste state than in powder and sheet states. The detail will be presented in the talk.

# In-Situ Study of Liquid-Liquid Phase Separation Behavior in Cu-Fe Alloys by Synchrotron X-ray Imaging

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## Abstract

Cu-Fe alloy is an immiscible alloy having a wide miscibility gap in the liquid phase with a high enthalpy of mixing. During the casting process after melting of the alloy, the undercooled liquid starts separation by producing Cu-rich liquid and Fe-rich liquid phases until reaching the nucleation temperature of Fe solid. It is assumed that these separated Fe-rich liquid droplets move and agglomerate, which gives rise to the typical egg-type microstructure. The motion of the liquid droplets is explained by the density difference between Cu and Fe elements and the temperature gradient in which the droplets move in the direction of reducing the interface energy.

It is necessary to understand the liquid-liquid phase separation behavior to prevent the agglomeration of droplets and ultimately make a uniform bimodal structure. In this study, for the first time, the liquid-liquid phase separation has been observed and successfully visualized in real-time with the synchrotron X-ray transmission imaging technique. The high energy and intensity of the beam have enabled the visualization of such a heavy metal alloy. The experimental setup, the imaging processing procedures, and the theoretical explanation of the movement of the droplets will be given in the presentation.

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*Keywords: Cu-Fe alloy, Liquid-liquid phase separation, Agglomeration, Synchrotron X-ray imaging, Image processing.*

# In-Situ SEM Observation Combined with DIC Strain Analysis for Understanding Deformation and Cracking in Metal Coatings

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## Abstract

Metal coatings are widely used to impart functionalities such as thermal, wear, and corrosion protection on the surface of engineering parts. To achieve sufficient formability of zinc (Zn) or aluminum (Al) alloy coated steel sheets, it is necessary to scrutinize the inhomogeneous deformation and its related crack initiation and propagation in the alloy coating layer. In-situ SEM observation combined with digital image correlation (DIC) strain analysis could be effective in quantifying the local strain distribution to investigate the cracking mechanism.

In this study, the microstructures of hot-dipped Zn-6Al-3Mg (wt.%) alloy coated steel sheets were successively observed using a miniature-sized 4-point bending test machine operated inside the SEM chamber. Captured in-situ SEM images were used for DIC strain analysis. The present Zn-Al-Mg alloy coating exhibited the solidification microstructure composed of a three-phase eutectic of fine Al (fcc), Zn (hcp), and $Zn_2Mg$ phases surrounding the primary solidified Al phases. No crack was found on the compressive-strained surface after the bending test, while parallel cracks were found on the tensile-strained surface of the Zn-Al-Mg alloy coating. In-situ SEM observation for the tensile-strained coating revealed that cracks were initiated on the surface of the Zn-Al-Mg alloy coating and then propagated inside of the coating. DIC strain analyses applied to the in-situ observed SEM images revealed the strain localization around the interface with the substrate steel sheets. The effect of the solidification microstructure on cracking behavior will be discussed utilizing the results of local strain quantified by DIC analysis.

*Keywords: Digital image correlation, In-situ observation, Plastic deformation, Cracking, Metal coatings*

# Study of crack propagation, dislocation movement and deformation twin evolution in Al-Sc alloy during in-situ TEM tension

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## Abstract

In-situ tension test in a transmission electron microscope (TEM) was used to study the fracture process of Al-Sc alloy, as well as the real-time crack propagation, dislocation movement and deformation twin evolution were captured. The results shows that microcracks are easy to form in the dislocation plugging zone in the crystal thinning zone, and then gradually expand to form large cracks during the fracture process of Al-Sc alloy. When $Al_3Sc$ particles exist in the crystal thinning region, microcracks first form on the surface of $Al_3Sc$ particles, and then the microcracks continue to expand and form fracture surface holes on the surface of the particles. Finally, the pore structure rapidly expands along the surface of the particles to form large cracks. The crack tip of Al-Sc alloy is always in a state of high stress and continues to emit dislocations into the matrix. The emitted dislocations form an intrinsic dislocation wall, which causes partial torsion of the crystals with the same orientation at the crack tip, and the torsion angle is inversely proportional to the mean dislocation distance. At the crack tip of the Al-Sc alloy, the deformation twin evolves by emitting thin twins into the interior of the matrix, and the emergence of incoherent twin boundaries is the main reason for the increasing thickness of the deformed twin. The slip of twin dislocations in the matrix leads to the change of orientation of the matrix atoms and the migration of twin boundaries.

*Keywords: Al-Sc alloy; In-situ TEM tension; Crack propagation; Dislocation movement; Deformation twin evolution.*

# Technical **Oral Session _ Session 3**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 3 (K3)** **16:00 -18:15, Nov. 20**

**Chair :** Koichi Tsuchiya (National Institute for Materials Science) Samda Hall B, 3F

16:00-16:30 **K-K0852** **[Keynote] Strength-ductility synergy via unusual deformation mechanism in HEAs**
En MA (Xi'an Jiaotong University, China)

16:30-16:50 **I-K1053** **[Invited] Enhancing mechanical properties of multi-principal element alloys through phase engineering**
Yujie Chen (University of Adelaide, Australia)

16:50-17:10 **I-K0704** **[Invited] Mechanical behavior of hetero-structured ferrous medium-entropy alloy**
Jae Wung Bae (Pukyong National University, Korea)

17:10-17:30 **I-K0822** **[Invited] A strong and ductile NiCoCr-based medium-entropy alloy strengthened by coherent nanoparticles with superb thermal-stability**
Jinyu ZHANG (Xi'an Jiaotong University, China)

17:30-17:45 **O-K0492** **Formation of ultra-fine-grained microstructure in CoCrFeMnNiAl high-entropy alloy by high-speed shear deformation followed by heat treatment**
Shunsuke Nakamura (Kobe University, Japan)

17:45-18:00 **O-K0695** **Low-cycle fatigue response of an equiatomic CrFeNi multi-principal element alloy**
Ankur Chauhan (Indian Institute Of Science, Bengaluru, India)

18:00-18:15 **O-K0599** **Tailoring microstructure and corrosion behavior of CoNiVAlx medium entropy alloys via Al addition**
Zhimin Pan (University of Science And Technology Beijing, China)

# Strength-ductility synergy via unusual deformation mechanism in HEAs

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We compare the strength, ductility and fracture toughness of NiCoCr MEA directly with those of a similar fcc alloy (316 strainless steel), and conclude that the MEA has yet to fully exploit the unusual dislocation mechanism (nanoscale segment detrapping, NSD) in HEA to drastically outperform known alloys. To expand further into new territory in the property space, we can take advantage of the vast possibilities of inhomogeneities in HEAs. In particular, the chemical inhomogeneity has two prongs that can be present separately, but sometimes co-exist: i) concentration fluctuation/undulation that can be intentionally enlarged and manipulated [1]); ii) local chemical order [2] that arises from the varying chemical affinity among the constitutent species. Both aspects further roughen the atomic and energy landscape, elevating cocktail hardening based on NSD. The resultant stick-slip makes it easy for the deformation carriers (dislocations and twins) to stall, multiply and accumulate, such that HEAs have an unusal ability to work-harden on the fly with increasing strain. These dynamic effects on defect evolution help delocalize the plastic strain, making it practical to achieve pure-metal-like ductility simultaneously with gigapascal yield strength, including in BCC refractory HEAs [3] that normally suffer from low tensile ductility.

[1] H. Li *et al.*, Nature, 604 (2022) 273-279;
[2] X. Chen *et al.*, Nature, 592 (2021) 712-716;
[3] L. Wang *et al.*, Nature Mater. (2023) April 10.

# Enhancing mechanical properties of multi-principal element alloys through phase engineering

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## Abstract

Phase structure plays a critical role in determining the mechanical properties of high-entropy alloys (HEAs). To further enhance the performance of metastable HEAs in load-bearing applications, a controllable synthesis with desired phases is required. In this work $(Fe_{49.5}Mn_{30}Co_{10}Cr_{10})N_x$ HEAs were prepared via magnetron sputtering, with the phase structure tuned by varying the nitrogen flow rate (i.e., $R_N$ = 4, 8, 10, 15, and 20 sccm). The phase structural evolution and mechanical properties of the new HEAs were investigated with a focus on the nitrogen addition. A solid solution consisting of single FCC phase was formed at lower $R_N$. With increasing $R_N$, a distinct transition in the alloy takes places; namely, first from FCC to FCC nanotwins and then to a mix of FCC and HCP, presumably instigated by the decrease of stacking fault energy. The new alloy prepared at $R_N$ = 15 sccm exhibits an ultrahigh hardness value of 21.5 GPa, and excellent damage tolerance. As such, our work offers a new metallurgy design route to exploring hitherto uncharted territory in the hardness-toughness space.

*Keywords: high-entropy alloys; magnetron sputtering; microstructures; hardness; damage tolerance*

# Mechanical behavior of hetero-structured ferrous medium-entropy alloy

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**Abstract**

High-entropy alloys (HEAs) and medium-entropy alloys (MEAs) have emerged as promising candidates for next-generation structural materials. Despite their remarkable mechanical performance, the practical implementation of these alloys is impeded by their high raw-material costs. To address this challenge, a novel class of non-equiatomic Fe-rich MEAs, referred to as ferrous medium-entropy alloys (FeMEAs), has been developed. The key strategy for the development of FeMEAs involves increasing the Fe content through the utilization of the pseudo-binary method, thereby enabling a cost-effective approach.

In this study, we present an overview of the design and mechanical behavior of FeMEAs as part of a transformative paradigm in HEA concept. We specifically focus on elucidating the crucial role of deformation mechanisms, which underlies the manifestation of favorable low-temperature mechanical properties. In addition, we emphasize the significance of tuning both chemical composition and microstructure to achieve controllable phase stability. Through this investigation, we aim to assess the potential development prospects for iron-based HEAs in future applications.

*Keywords: High-entropy alloys, Ferrous medium-entropy alloys, transformation-induced plasticity, low-temperature tensile properties, hetero-structuring*

# A strong and ductile NiCoCr-based medium-entropy alloy strengthened by coherent nanoparticles with superb thermal-stability

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**Abstract:** In this work, we designed a novel NiCoCr-based medium-entropy alloy (MEA) strengthened by coherent $L1_2$-nanoparticles, *i.e.*, $(NiCoCr)_{92}Al_6Ta_2$ (at.%). The strengthening and deformation mechanisms of the material and the coarsening kinetics of the coherent precipitates were systematically investigated. The results indicated that giant precipitation hardening and its synergy with other strengthening contributors confer on the aged material a yield strength as high as 1.0 GPa. Moreover, a unique particle-features-dependent plasticity mechanism was revealed in this alloy. That is, the alloy with a lower volume fraction, denser-distribution and finer particles mainly deformed by dislocation planar slip, otherwise, stack-faults-mediated plasticity was favored, rationalized by the cooperative/competitive effect of stack-fault energy, spatial confinement and applied stress. Furthermore, the coarsening behavior of precipitate followed a modified LSW model, and the nanoparticles displayed remarkably superior thermal-stability compared to most traditional superalloys and reported multicomponent alloys. The superb coarsening resistance of precipitate originated from the coupled-effect of intrinsic sluggish diffusion in multi-principal alloys and the dual-roles of Ta species as a precipitate stabilizer. This work provides a new pathway to develop strong-yet-ductile multicomponent alloys as promising candidates for high-temperature applications.

*Keywords: Medium-entropy alloy, mechanical properties, precipitation hardening, deformation mechanisms, coarsening kinetics.*

# Formation of ultra-fine-grained microstructure in CoCrFeMnNiAl high-entropy alloy by high-speed shear deformation followed by heat treatment

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## Abstract

Recently, High-entropy alloy (HEA) has been expected to be used for structural applications. CoCrFeMnNi has been of particular interest, and it has been shown that the addition of Al improves the strength by forming FCC/BCC dual-phase structure and distributing hard sigma phase precipitates after heat treatment. The purpose of this study is to elucidate the formation mechanism and condition of the recrystallized microstructure of $Al_{0.5}$CoCrFeMnNi alloy with FCC/BCC dual-phase structure, which is formed by high-speed shear deformation followed by heat treatment. Submicron-order FCC grains were formed in shear bands by static recrystallization after the severe shear deformation followed by heat treatment at 1023 ~ 1123 K. In addition, a high number density of precipitates of the BCC and sigma phase were observed in the shear band region. The hardness difference with the FCC matrix suggests that the formation of FCC fine grains is due to the grain boundary pinning effect by the hard phase precipitates. In addition, there was a region where FCC fine particles were not formed in the shear zone. A possible reason for this difference is the change in the amount of strain accumulated in the shear localized region. Comparing the equivalent strain distributions obtained by finite element analysis, it was predicted that there would be a difference in the amount of strain introduced between the fine-grained FCC regions and the coarse-grained regions. Therefore, the experimental results show that the introduction of certain level of strain is necessary for the formation of shear bands and subsequent FCC grain refinement after heat treatment.

*Keywords: High Entropy Alloy, Severe plastic deformation, Shear band, Precipitation, Grain refinement*

# Low-cycle fatigue response of an equiatomic CrFeNi multi-principal element alloy

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## Abstract

For multi-principal element alloys (MPEAs) potential engineering applications, understanding their low-cycle fatigue (LCF) behavior is of decisive importance. Recently, an equiatomic face-centered cubic (FCC) CrFeNi has been shown to offer an excellent combination of monotonic properties. In the present study, we report on its LCF behavior at room temperature. Fully reversed strain-controlled fatigue tests were conducted in air under three different strain amplitudes (± 0.3%, ± 0.5% and ± 0.7%). The measured cyclic stress response reveals a rapid increase (i.e., cyclic hardening) followed by a relatively gradual decrease of peak stresses (i.e., cyclic softening) until failure. Electron microscopy investigations on post-fatigue samples revealed strain amplitude dependent dislocations slip-modes and resulting substructure evolutions. These observations are linked to the observed cyclic stress response and lifetime. Furthermore, the origin of CrFeNi's cyclic stress response is analyzed by partitioning hysteresis loops. Lastly, a comparison with similar grain-sized (60-67 µm) CoCrFeMnNi, and 316L alloys pinpoints the peculiarities of CrFeNi LCF response, which is discussed in terms of the difference in their solid solution strengthening, grain boundary strengthening and stacking fault energy.

*Keywords: High-entropy alloys; Low-cycle fatigue; Dislocation structures; Effective stress; Back stress.*

# Tailoring microstructure and corrosion behavior of $CoNiVAl_x$ medium entropy alloys via Al addition

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## Abstract

The effect of Al addition on the microstructure and corrosion behavior of $CoNiVAl_x$ medium entropy alloys (MEAs) was investigated. Results indicated that increasing Al addition leaded to the increase in the atomic ratio of Al/V and $O^{2-}/OH^-$, which implied that Al addition promoted the increase of metallic oxide in the film, thus enhancing the stability and protection of the passive film. The enhanced corrosion resistance caused by Al addition might be attributed to the dominant role of Al in stabilizing the passive film. The difference in the Volta potentials of FCC and BCC phases indicated the existence of microgalvanic coupling, which suggested that the BCC phase served as a localized cathode while the FCC matrix and FCC lath acted as anodes. This accounted for the pitting mechanism of $CoNiVAl_x$ MEAs via Al addition. The current work can provide some guidance in assessing the corrosion resistance of alloy systems containing precipitates.

*Keywords: Medium entropy alloy; Corrosion resistance; Microstructure; Precipitate; Passive film.*

# Technical **Oral Session _ Session 3**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 3 (L3)** **16:00 -18:05, Nov. 20**

**Chair :** Je In Lee (Pusan National University) 202B, 2F

16:00-16:20 **I-L0672** **[Invited] Local Strain Distribution and Microstructure around Al3Ti Platelet Particle in Al-Al3Ti Composite**
Hisashi Sato (Nagoya Institute of Technology, Japan)

16:20-16:35 **O-L1006** **Improved mechanical properties of nacre-like (TiBw+TiB2)/2024Al composites fabricated by freeze casting and T6 heat treatment**
Jidong Zhang (Harbin Institute of Technology, China)

16:35-16:50 **O-L0463** **Investigating the Effect of Processing Parameters on the Morphology and Properties of PA6/carbon Fiber Composites for Overmolding Applications**
Gu-Hyeok Kang (Fraunhofer-Institut Für Chemische Technologie, Germany)

16:50-17:05 **O-L0913** **Significantly Refined Microstructure of TiBw/TA15(Si) Composites by Single-Pass Hot Pressing with Prior Heat-treatment**
Rui Zhang (Harbin Institute of Technology, China)

17:05-17:20 **O-L0100** **Deformation and aging behaviours of the single crystal Ni-Mn-Ga particles/silicone rubber towards magnetic field driven actuators**
Wan-Ting CHIU (Tokyo Institute of Technology, Japan)

17:20-17:35 **O-L0050** **Study on interface bonding and wear resistance of rare earth doped WC Iron Matrix Composites**
Wengao Zhang (Kunming University of Science and Technology, China)

17:35-17:50 **O-L0645** **Investigation on the elevated temperature tribological behavior of in-situ sub-micron/nano magnesium matrix composite**
Sushanta Kumar Sahoo (Indian Institute of Technology Madras, India)

17:50-18:05 **O-L1002** **Effect of SiCnp addition on microstructure and mechanical properties of graphene nanosheet (GNS) reinforced aluminum composites**
Jiajia Zhang (Harbin Institute of Technology, China)

# Local Strain Distribution and Microstructure around $Al_3Ti$ Platelet Particle in Al-$Al_3Ti$ Composite

**Hisashi Sato**[1], Makoto Kikko[2], Mami Mihara-Narita[3], Yoshimi Watanabe[4]

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## Abstract

Al-Based composite containing Al-Ti intermetallic compound as reinforcement is expected to be applied as airplane materials because of its high strength and light weight. Moreover, it is known that this composite has good lattice matching between the matrix and the reinforcement, and that Al-$Al_3Ti$ composite containing $Al_3Ti$ platelet particles has been used as grain refiner of as-cast Al. This is because the $Al_3Ti$ particles in the Al melt play a role of heterogeneous nucleation site of Al. From the microstructural characteristics of the Al-$Al_3Ti$ composite, the Al matrix in the Al-$Al_3Ti$ composite would have local elastic strain around the $Al_3Ti$ platelet particle. However, the distribution of the local elastic strain in the Al matrix around the $Al_3Ti$ platelet particle is unclear. Recently, elastic strain measurement technique using electron backscatter diffraction (EBSD-Wilkinson method) has been proposed. The EBSD-Wilkinson method can visualize elastic strain distribution in a grain. In this study, the local elastic strain distribution of the Al around an $Al_3Ti$ platelet particle in the Al-$Al_3Ti$ composite is investigated using the EBSD-Wilkinson method. The elastic strain distributions were evaluated around two large Al/$Al_3Ti$ interfaces. One interface has crystal orientation relationship of $(001)_{Al}//(001)_{Al3Ti}$, $[100]_{Al}//[100]_{Al3Ti}$ and the other one has that of $(221)_{Al}//(001)_{Al3Ti}$, $[11{-}1]_{Al}//[210]_{Al3Ti}$. The elastic strain in the Al matrix at the later interface is larger than that at the former interface. Moreover, this elastic strain is distributed along the later interface. Based on these results, microstructural formation around the $Al_3Ti$ platelet particle is discussed.

*Keywords: Al-$Al_3Ti$, Residual Strain, Electron backscattering diffraction (EBSD), Crystal Orientation Relationship*

# Improved mechanical properties of nacre-like ($TiB_w$+$TiB_2$)/2024Al composites fabricated by freeze casting and T6 heat treatment

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Abstract

The bio-inspired ($TiB_2$+TiBw)/2024Al composites with lamellar structure were prepared through freeze casting combined with squeeze casting, and the mechanical properties of the composites were improved by T6 heat treatment. The influence of the T6 heat treatment on the microstructure evolution and mechanical properties of the bio-inspired ($TiB_2$+TiBw)/2024Al composites was systematically investigated. The results illustrated that the introduction of the lamellar structure inhibited the dissolution of the second phase and accelerated the ageing behavior of the Al matrix reducing the duration of peak aging. The reduction in aging time can be attributed to the dislocation resulting from the mismatch in thermal expansion coefficients between the reinforcements and the Al matrix. Both the optimum solution condition and aging condition was determined to be 510 °C for 2 h and 160 °C for 16 h respectively, with the superior compressive strength of 886 MPa, bending strength of 710 MPa, and crack propagation toughness of 36 $MPa.m^{1/2}$. The excellent mechanical properties are ascribed to the particularly nacre-like structure, which prevents Al matrix deformation, inhibits dislocation movement and increases the crack propagation path.

**Keywords:** freeze casting; bio-inspired ($TiB_2$+TiBw)/2024Al composites; in-situ reaction; T6 heat treatment

# Investigating the Effect of Processing Parameters on the Morphology and Properties of PA6/carbon Fiber Composites for Overmolding Applications

**Gu-Hyeok Kang[1]**, Christoph Schelleis[1], Björn Beck[1], Michael Wilhelm[1], Frank Henning[1]

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## Abstract

The study investigates the overmolding process of a carbon fiber-reinforced polyamide 6 (PA6) composite into a glass fiber-reinforced PA6 profile using the in-situ polymerization pulse method. The objective of the study is to optimize the processing parameters to achieve desired mechanical characteristics, including tensile strength, bending strength, impact strength, and modulus in each test. The effects of molding pressure, carbon fiber content, treatment temperature, and fiber surface treatment in both the in-situ polymerization and overmolding processes were examined as shown in the Fig 1 and 2.

To achieve a high weight percentage profile, the paper utilizes a monomer caprolactam and a catalyst through pultrusion and ring-opening polymerization processes. Overmolding is performed using injection molding, where a composite material reinforced with chopped carbon fiber and PA6 serves as the matrix. The research emphasizes the importance of high interfacial adhesion, physical properties, low cost, low environmental impact, and shape flexibility.

The study's results indicate that Young's modulus tends to increase with a higher carbon fiber content, with a peak Young's modulus of 1.8 GPa observed at a content of 24 wt%. However, the properties of the moisture-absorbing specimens decreased to 1.3 GPa when exposed to an environment simulating atmospheric humidity.

Furthermore, the use of a monomer caprolactam and a catalyst in the manufacturing process ensures cost-effectiveness in producing high weight percentage profiles. The research also highlights the potential of employing a composite material reinforced with chopped carbon fiber and PA6 as the matrix, offering advantages such as low environmental impact and design freedom. These findings contribute to the development of new high-performance composite materials that can meet diverse industry needs.

**Acknowledgement**- This research was supported by the Materials/Parts Technology Development Program (Grant No. 20010515) funded by the Ministry of Trade, Industry and Energy (MOTIE) of Korea through Korea Evaluation Institute of Industrial Technology (KEIT).





Fig. 1. Overmolding flow progress (left) and Fig. 2. Overmolding on a pultruded profile (right)

*Keywords: PA6, Pultrusion, Overmolding,*

# Significantly Refined Microstructure of TiBw/TA15(Si) Composites by Single-Pass Hot Pressing with Prior Heat-treatment

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## Abstract

Titanium matrix composites (TMCs) have good mechanical properties at elevated temperatures, but the ductility at room temperature and formability are unsatisfactory. In the present work, the hot processing procedure of TiBw/TA15(Si) composite is studied and optimized to achieve a refined microstructure. The composite was first heat-treated above β transformation temperature, and then hot-pressed at 920 °C. An equiaxed microstructure was obtained after the deformation. A comparison with the composite subjected only to hot pressing revealed that the prior heat treatment led to a more refined and homogeneous microstructure. The size of α grains was reduced from ~5 μm to ~2 μm, and the size of silicide particles decreased to below 100 nm. The deformed composite demonstrated a strength of 1120 MPa and ductility of 7%, both of which can be further improved by heat-treatment. Additionally, the hot-pressed composite exhibited superplastic behavior at elevated temperatures, achieving a tensile elongation of 310% at 800 °C, which is four times higher than that of the as-sintered composite. Further analysis indicates that the refinement of α grains and dispersed distribution of silicide particles significantly contribute to room temperature strengthening, while the improved high-temperature deformability is attributed to the triggering of the grain-boundary sliding mechanisms by the refined and equiaxed microstructure.

*Keywords: Titanium matrix composites; heat-treatment; hot processing; microstructure refinement.*

| O-L0100 |

# Deformation and aging behaviours of the single crystal Ni-Mn-Ga particles/silicone rubber towards magnetic field driven actuators

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## Abstract

Shape change of the ferromagnetic shape memory alloys (FSMAs) is manipulatable via applying a magnetic field [1]. The Ni-Mn-Ga-based alloys are considered as promising FSMAs for the applications as magnetic field-driven devices; however, their high brittleness and limited shape change due to the grain boundary constraints are challenging factors for their practicability. To overcome these shortcomings, in this work, the single crystalline Ni-Mn-Ga particles were integrated into silicone rubber.

For operating as a magnetic field driven actuator, the shape change characteristics of the Ni-Mn-Ga/silicone composite were studied under an external magnetic field. A giant magnetic field induced strain (MFIS) of 4% under a magnetic field of around 1 T was obtained in the as-prepared composite [2]. It was found that such MFIS was reproduced with only 5% of decline after 5-years storage of this composite material. It is thus confirmed that the composite materials possess a high resistance to the aging effect in terms of the shape change driven by an external magnetic field. Additionally, cyclic examinations conducted under compressive stress and magnetic field were performed to confirm cyclic stability of deformation behaviour of these composites.

References:

[1] V.A. Chernenko, Magnetostrictive Ni-Mn-Based Heusler Alloys in *Encyclopedia of Smart Materials*. (ed. Olabi, A.G.) 160-176, Elsevier, 2022.

[2] W.T. Chiu, P. Sratong-on, M. Tahara, V. Chernenko, H. Hosoda, *Scr. Mater.* 207 (2022) 114265.

*Keywords: Ferromagnetic shape memory alloys, Magnetic field driven actuators, Ni-Mn-Ga/silicone Composites, Shape memory alloys*

# Study on interface bonding and wear resistance of rare earth doped WC Iron Matrix Composites

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**Abstract**

WC particle reinforced iron matrix composites have a broad application prospect in the field of wear resistance. In this paper, rare earth elements such as Nd and Y were selected to prepare rare earth doped WC iron matrix composites by powder metallurgy. The effects of rare earth elements (Nd, Y, Ce, La) doping on interface properties were calculated by first principles, and the microhardness and wear properties were tested respectively. The results show that the doping of rare earth elements strengthens the charge transfer between Fe, W and C atoms at the interface, strengthens the bonding between atoms, and increases the bonding strength at the interface. In addition, the binding strength of rare earth Nd doped interface is the best, and Nd element can be optimized to modify the interface. The addition of Nd reduces the hardness of the interfacial reaction zone from 1375.5HV to 1167.9HV, but the hardness of the matrix increases from 132.8HV to 177.3HV. The wear resistance of rare-earth doped composite is higher than that of undoped rare-earth composite mainly because the strength and hardness of the composite are enhanced by rare-earth elements. The above results have important guiding significance for improving the strength and wear resistance of WC iron matrix composites.

*Keywords: WC iron matrix composites, Adhesion work, Rare earth, Wear resistance.*

# Investigation on the elevated temperature tribological behavior of in-situ sub-micron/nano magnesium matrix composite

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## Abstract

The development of new structural materials with high strength-to-weight ratios poses significant challenges in the automotive industry, aiming to reduce fuel consumption and greenhouse gas emissions. Magnesium (Mg) matrix in-situ reinforced composites are exceptional engineering materials due to their remarkable specific strength, young's modulus, and wear resistance. Currently, there is extensive exploration of magnesium-based composites for high-temperature applications, including automotive engine parts, oil pump covers, cylinder liners, aircraft engine casing and various wear-resistant applications. The present investigation is focused to study the high temperature tribological performance of a rare-earth contained Mg alloy with and without in-situ $TiB_2$ reinforcement. The impact of in-situ $TiB_2$ particles on different wear mechanisms, such as abrasive wear, plastic deformation, oxidation, delamination, and melt wear was studied in detail. Wear mechanism maps were constructed by correlating the worn surface microstructural features with the wear test parameters. These maps facilitated the identification of optimal transition wear parameters from mild to severe wear conditions. The scientific knowhow on tribological behavior of ZE41 Mg alloy with/without in-situ $TiB_2$ particles was established via understanding the governing dominant high temperature wear mechanisms.

*Keywords: Magnesium Matrix Composite; Sub-micron/nano In-situ Reinforcement; Tribological Behavior; Elevated Temperature; Wear Mechanism Map*

# Effect of SiCnp addition on microstructure and mechanical properties of graphene nanosheet (GNS) reinforced aluminum composites

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## Abstract

Homogeneous dispersion of high-content GNS is the challenge and key to achieve high mechanical properties of graphene reinforced aluminum matrix composites (GNS/Al). In traditional methods, the homogeneous dispersion of GNS is often achieved by prolonging the ball milling time or increasing the ball milling energy, which is often accompanied by severe damage to GNS structure. Here, a two-step ball milling process was employed to introduce SiC nanoparticles (SiCnp) in GNS/Al composites, which improves the GNS distribution while also playing an additional strengthening role. The Al flakes with a large lateral to thickness ratio were produced by a first-step ball milling of SiCnp and Al powders. The obtained Al flakes effectively improved the dispersion efficiency of GNS and reduced the GNS structural damage. As a consequence, GNS and SiCnp were well dispersed and combined with Al matrix after hot extrusion. The nanograins were also obtained in the extruded (GNS+SiCnp)/Al composites, which were conducive to the strengthening of composites. Benefiting from the homogeneous dispersion of GNS, SiCnp and the hybrid enhancement effect between them, the ultimate tensile strength (UTS) and elongation of the extruded (GNS+SiCnp)/Al composites were increased by 41.0% and 47.6% compared with GNS/Al composites, yielding good comprehensive mechanical properties.

*Keywords: aluminum-matrix nanocomposites; two-step ball milling; hybridization effect; spark plasma sintering (SPS)*

# Technical **Oral Session _ Session 3**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 3 (M3)** **16:00 -17:55, Nov. 20**

**Chair :** Yuntian Zhu, City University Of Hong Kong
Ju-Young Kim, Ulsan National Institute of Science and Technology
402, 4F

16:00-16:30 **K-M0696** **[Keynote] On nanoindentation of severe plastic deformation processed structural alloys**
Jae-il Jang (Hanyang University, Korea)

16:30-16:50 **I-M0559** **[Invited] Ultra-sensitive thin film metal crack sensor for reliability assessmen**
Seung-Kyun Kang (Seoul National University, Korea)

16:50-17:10 **I-M0354** **[Invited] Characteristic Lengths of Nanostructured Metals observed in Atomic Simulations**
Tomotsugu Shimokawa (Kanazawa University, Japan)

17:10-17:25 **O-M1022** **Ultrafine-grained AZ61 alloy produced by high-pressure sliding**
Intan Fadhlina Mohamed (Universiti Kebangsaan Malaysia, Malaysia)

17:25-17:40 **O-M1117** **Recent Advancements in Constrained Groove Pressing Process**
Sunil Kumar (S. V. National Institute of Technology Surat, Indian)

17:40-17:55 **O-M1110** **Fabrication and characterization of ultrathin copper foils by accumulative pack rolling process**
Ning Nie (University of Wollongong, Australia)

# On nanoindentation of severe plastic deformation processed structural alloys

Zhe Gao[1], Dong-Hyun Lee[2], In-Chul Choi[3], **Jae-il Jang[4]**

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**Abstract**

Over the past 3 decades since it was first introduced in 1980s, nanoindentation technique has been widely used to estimate the various mechanical properties of the small volume in a material at much smaller loads and size scales than conventional (micro-)hardness tests. Now, the technique is being considered not only as a characterizing tool but as a promising technology for better understanding of the mechanisms of small-scale mechanical/physical behavior from materials science viewpoints. In this talk, based on the research of my group and colleagues, I would like to introduce the recent nanoindentation studies performed on severe plastic deformation (SPD) processed structural alloys, which can be a good example to show how this becoming-somewhat-old technique can be still powerful tool for developing novel structural materials.

*Keywords: Nanoindentation, severe plastic deformation, structural materials, nanomechanics, hardness.*

# Ultra-sensitive thin film metal crack sensor for reliability assessment

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## Abstract

Cracks in metallic materials can serve as a highly useful tool for adjusting the distance of electrical bonds at an atomic level. Even slight opening of tiny cracks can lead to significant variation in electrical conductivity. Recently, the feature of micro-cracks that can convert mechanical deformation into sensitive electrical signals has been utilized in the development of highly sensitive thin-film strain sensors, also known as metal crack-based strain sensor technology. It has been receiving attention for its excellent sensitivity and flexibility with very simple structure. In this study, we aim to introduce a technology that can control the sensitivity and measurement range of the strain sensor by utilizing metamaterials capable of converting the mechanism by which micro-cracks expand. Through a substrate that incorporates a combination of various Poisson's ratios, including negative ones, we can freely adjust the rate of change in sensitivity. Furthermore, we aim to discuss applications that can provide preemptive diagnosis of cracks occurring inside pipelines by combining wireless communication technology.

*Keywords: metal crack sensor, ultra-sensitive strain sensor, meta materials, negative Poisson's effect, reliability*

# Characteristic Lengths of Nanostructured Metals observed in Atomic Simulations

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## Abstract

Nanostructured metals produced by severe plastic deformation have been reported to exhibit unique mechanical properties. With the refinement of microstructures, the spatial scale in which dislocations can move becomes smaller, and the volume fraction of surface defects increases. The former affects the inhomogeneity of the mechanical field via elastic interactions between dislocations, and the latter results in a larger contribution of plastic deformation phenomena via plane defects. These co-operative phenomena of the development of lattice defects result in the emergence of characteristic lengths with respect to mechanical properties, and these characteristic lengths are considered to be strongly influenced by the structure and morphology of the plane defects. In this study, we investigate the characteristic length for strength in nanostructured materials using atomistic simulations that can directly represent lattice defect dynamics and plane defect structures. Two models are analyzed: one is a polycrystalline model consisting of cubic grains, and the other is a single-crystal model containing deformed twins. In the former, tensile and shear deformation are applied perpendicular to the grain boundary, respectively, and the grain size dependence of strength is examined. In the latter model, dislocations are piled up on the deformation twin and the thickness dependence of the strength when the dislocations pass through the deformation twin is investigated. Through these atomic simulations, we discuss the characteristic length of nanostructured materials with respect to strength.

*Keywords: Size effect, Mechanical property, Molecular dynamics analysis, Grain boundary, Deformation twin*

# Ultrafine-grained AZ61 alloy produced by high-pressure sliding

**Intan Fadhlina Mohamed**[1], Ahmad Muhammad Aziz[2], Zenji Horita[3,4,5,6]

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**Abstract**

In this study, an AZ61 Mg alloy was processed by high-pressure sliding (HPS) for grain refinement. The HPS process was carried out at room temperature under 4 GPa for a sliding distance of 15 mm at a sliding speed of 1.0 mm/s using rectangular sheets with 100 mm length and 10 mm width. Tensile tests were carried out at elevated temperatures and microstructures were observed by transmission electron microscopy (TEM). The grain size was well reduced to ~1.72 μm after HPS processing. This reduction in the grain size led to superplastic elongation of ~510% at 573 K with an initial strain rate of $5.5 \times 10^{-4}$ $s^{-1}$. The results were then compared with those obtained using the Incremental Feeding HPS(IF-HPS). The result shows the presence of superplastic behaviour in IF-HPS with an appreciable total elongation of ~320%. Thus, it can be concluded that AZ61 was successfully processed by HPS including the upscaling IF-HPS process.

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*Keywords: High-pressure sliding, AZ61, superplasticity*

# Recent Advancements in Constrained Groove Pressing Process

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## Abstract

Among various severe plastic deformation (SPD) techniques, constrained groove pressing (CGP) has arisen as a famous technique for fabricating ultrafine-grained sheet metals and alloys in recent times. The severe strain is applied to improve the mechanical performance and properties. However, inhomogeneous grain refinement, lower formability, surface unevenness, and microcracks are the common limitations of conventional CGP-processed samples. Therefore, the latest progress to overcome such limitations and comparison of process efficacy with the conventional process will be highlighted through various advanced CGP processing techniques, such as modification of die design, annealing of the processed sample, cross CGP, ring CGP, hybrid SPD, covered sheet casing CGP, and rubber pad CGP. All techniques are emerging to upscale the procedure and improve grain refinement through various approaches, producing superior mechanical properties. The historic research of conventional CGP and its effect on grain refinement and mechanical properties will be initially briefed and then recent progress through different advanced techniques will be highlighted, especially in alloys.

*Keywords: Constrained Groove Pressing, Ultra-fine grain, Mechanical Properties, Grain Refinement.*

# Fabrication and characterization of ultrathin copper foils by accumulative pack rolling process

**Ning Nie[1],** Lihong Su[1], Rui Wang[1], Kiet Tieu[1], Huijun Li[1]

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## Abstract

Copper foils have been widely used in electronic industry owing to their advantages of excellent conductivity, chemical resistance and good balance of strength and flexibility. With ever increasing interests in the fields of mobile phone, wireless broadband network and flexible electronics, copper foils are often used for current collectors, printed wiring boards, printed circuit boards and flexible printed circuit boards. These applications always require excellent surface quality, low-cost and ease of manufacturing for the copper foils. Cold rolling and electrodeposition are two main processes for the fabrication of copper foils. However, the surface roughness of copper foils fabricated using these methods is a challenge and an extra roughening treatment is always required. In this study, we have proposed an accumulative pack rolling (APR) process to manufacturing ultrathin copper foils with greatly improved efficiency. A minimum thickness of 2.2 μm can be obtained after the APR process. The microstructure and surface morphologies evolutions during APR process, and the effect of rolling direction have been comprehensively investigated.

*Keywords: Advanced manufacturing; Accumulative pack rolling; Copper foils; Microstructure; Surface roughness.*

# Technical **Oral Session _ Session 3**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 3 (N3)** **16:00 - 17:45, Nov. 20**

**Chair :** Dezhen Xue (Xi'an Jiaotong University) 203, 2F
Seunghwa Ryu (Korea Advanced Institute of Science and Technology)

16:00-16:30 **K-N1099** **[Keynote] Constitutive modelling based on machine learning for anisotropic plasticity**
Jeong Whan Yoon (KAIST/Deakin University, Korea)

16:30-16:45 **O-N1147** **Application of Thermodynamic extremal principle to Phase Field Model for Non-equilibrium Interface Conditions**
Yue Li (Northwestern Polytechnical University, China)

16:45-17:00 **O-N0270** **Application of finite element simulations to nanosecond laser ablation process**
Yutaka Tsumura (The University of Sydney, Australia)

17:00-17:15 **O-N0175** **Finite element simulation of plastic flow in dealloyed heterogeneous materials**
Sylvain Dancette (CNRS, Tohoku University, Japan)

17:15-17:30 **O-N0126** **Crystal Plasticity Simulation Considering Microstructures of Metals on Mechanical Anisotropy Induced by Rolling**
Nomun Gerel-Erdene (Tohoku University, Japan)

17:30-17:45 **O-N0678** **A physics-constrained ANN model for material deformation modelling**
Guowei Zhou (Shanghai Jiao Tong University, China)

# Constitutive modelling based on machine learning for anisotropic plasticity

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## Abstract

This study proposes a machine learning-based constitutive model for anisotropic plasticity in sheet metals. A fully connected deep neural network is constructed to learn the stress integration procedure under the plane stress condition. The DNN utilizes the labelled training data for feature learning, and the respective dataset is generated numerically based on the Euler-backward method for the whole loading domains with one element simulation. The DNN is trained sufficiently to learn all the incremental loading paths of the input-output stress pair by using advanced anisotropic yield functions. Its performance with anisotropy is evaluated for the predictions of r-values and normalized yield stress ratios along 0-90 degrees to the rolling direction. In addition, the trained DNN is then incorporated in user material subroutine UMAT in ABAQUS/Implicit. Thereafter, the DNN-based anisotropic constitutive model is tested with a cup drawing simulation to evaluate earing profile. The obtained earing profile is compatible with the one from the trained anisotropic yield function.

*Keywords: Deep Learning, Artificial Neural Network, Constitutive Model, Anisotropy, Finite Element Analysis*

# Application of Thermodynamic extremal principle to Phase Field Model for Non-equilibrium Interface Conditions

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## Abstract

Based on the thermodynamic extremal principle, this article presents a new phase-field formulation for non-equilibrium interface conditions in rapid phase transformations. With a particular way of defining concentration fields, the classical sharp and diffuse (thick) interface theories are unified into the present phase-field model. Each point inside the diffuse interface is comparable to the classical sharp interface model, governed by phase boundary migration and short-range atomic exchanges and connected by long-range diffusion. Their thermodynamic forces and fluxes are following the Onsager's reciprocal relation and consistent with the classical irreversible thermodynamics. Furthermore, we establish the balance of driving forces and energy dissipations for both the diffuse interface and the single point inside it, providing new understanding of interface thermodynamics and kinetics.

Topic area: Computational Materials and Artificial Intelligence (N)

*Keywords: Phase field, Thermodynamic extremal principle, Interface kinetics*

# Application of finite element simulations to nanosecond laser ablation process

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**Abstract**

Surface preparation of steelwork for structural repainting is often conducted by sandblasting method in which abrasives (sands) are blasted onto the painted surface at high speed, removing the old paint and rust/dirt from the impact of the blast. This conventional method would cause damage to the underlying substrate, deteriorating its mechanical and fatigue performance. Laser cleaning is an application of a laser ablation process, and it has attracted attention as an alternative to conventional cleaning methods as an environmentally friendly and economical technology that removes paint and corrosion efficiently. Laser material processing often involves strong non-linearity attributed to significant temperature change, material property changes and phase transformation. This can cause heat-related physical and/or chemical damages at the surface of the metal which could induce, crack formation, flaking from the surface and annealing/softening due to change in the residual stresses. It is necessary to carefully select the laser parameter such that any unwanted damage is minimized.

Selecting laser parameters generally involves enormous overhead as it is essentially a try-and-error method that requires multiple tests for a given application and a given material. Adding to this, the fact that the residual stress measurement using X-ray diffraction or neutron diffraction is costly which often limits the number of samples that can be tested experimentally.

This research investigates the mechanical properties in particular residual stresses of the laser ablated steel samples using finite element modelling. to better understand the changes in residual stress distribution and material properties. The model presented here incorporates a physical and mathematical model required to handle complex multi-physics phenomena, such as laser-substance interactions, thermal-mechanical interactions between melt pool and solid, and melting and re-solidification processes. Using this finite element model, simulations were run to determine the region in the material that is subjected to phase transformation and to determine how residual stresses change in the steel during laser ablation. Experimental measurements are also carried out to benchmark the model. Laser ablation using a nanosecond laser was performed on steel plates. The plates were then tested using X-ray diffraction for residual stress testing, and microstructure characterization was performed using a scanning electron microscope. A comparison between the finite element model and the experimental results is also presented.

# Finite element simulation of plastic flow in dealloyed heterogeneous materials

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**Abstract**

Liquid Metal Dealloying (LMD) is a recent method allowing to produce bicontinuous metal-metal composites or the corresponding porous foams, when one of the metallic phases is removed by chemical etching for example. The length scale of the ligaments in the microstructure can range from the nanometer to the micrometer range depending on process parameters. Another length scale in the microstructure is that of the grains, defining regions of a given crystallographic orientation in the material and also ranging from the (sub-)micron scale to potentially several hundreds of micrometers. In this work, the interplay between these two lengthscales is explored, focusing on the consequences on the anisotropy of mechanical properties. A numerical simulation framework is developed, allowing to generate finite element models representative of the dealloyed materials and to compute the heterogeneous mechanical behavior. A few examples of application are illustrated, from bulk microporous foams to core-shell particles with a dealloyed nanoporous shell structure.

*Keywords: nanoporous materials, liquid metal dealloying, finite element simulation, crystal plasticity.*

# Crystal Plasticity Simulation Considering Microstructures of Metals on Mechanical Anisotropy Induced by Rolling

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## Abstract

The rolling process, which has a low environmental impact yet can increase the strength of metallic material, has recently been studied since it has become difficult to expect these demands from the conventional metal strengthening methods such as alloying and heat treatment. However, it is known that mechanical anisotropy occurs in rolled metals. Rolling texture causes oriented distribution of the Schmidt factor, and dislocation density distribution yields critical resolved shear stress distribution, resulting in mechanical anisotropy and decreasing plastic forming accuracy. Our approach is to develop a method that reproduces mechanical anisotropy considering the crystal orientation and dislocation density. The degree of orientation is determined quantitatively by evaluating the orientation of the rolled microstructure. Resolved shear stress (RSS) estimated by the crystal orientation information measured by EBSD measurement predicts the dislocation density corresponding to the crystal orientation. Considering the dislocation density distribution for each slip system and the rolling texture based on the degree of orientation, crystal plasticity finite element simulations are performed to reproduce the mechanical anisotropy of rolled metal. The effectiveness of this method is verified by comparing the results with those of conventional analysis methods.

*Keywords: Finite Element Method, Mechanical Anisotropy, Crystal Plasticity Simulation, Rolling, Dislocation Density Distribution*

# A physics-constrained ANN model for material deformation modelling

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## Abstract

The Machine learning based modelling methods, especially the artificial neural network (ANN), has gained increasing popularity in the field of material science. In the current work, an artificial neural network-coupled crystal plasticity (ANN-CP) method considering physics-constrains is proposed to predict the mechanical response of face-centered cubic crystals under plain stress loading with arbitrary orientations in the entire Euler space. The physics-constrains in crystal plasticity are considered in the feature generation, loss function and data augmentation. The shear strain rate on each slip system identified as the key feature. Compared with the conventional feature selection and loss function, the proposed physics-constrained neural network accelerates model convergence and promotes prediction accuracy, especially for small-scale dataset. The proposed model can he complex in-plane deformation of crystals with any initial orientations, including cyclic loading and arbitrary non-monotonic loading.

*Keywords: Crystal plasticity, Machine learning, Neural networks, Physical constraints, Complex loading*

# Technical **Oral Session _ Session 3**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 3 (O3)** **16:00 - 17:10, Nov. 20**

**Chair :** Hong Luo (University of Science And Technology Beijing) 401, 4F

16:00-16:20 **I-O0374** **[Invited] Development of hydrogen embrittlement resistant high-strength steel based on deep hydrogen trap design**
Jing Liu (Wuhan University of Science and Technology/ ShenZhen University, China)

16:20-16:40 **I-O0771** **[Invited] The use of secondary resources in steel manufacturing**
Samane Maroufi (University of New South Wales, Australia)

16:40-16:55 **O-O0639** **Effect of ratio of scrap to iron source on slag-metal reactions in smelting and reduction process of iron ore**
Kengo Kato (University of Toyama, Japan)

16:55-17:10 **O-O0763** **Effect of gangue oxide in HBI on dephosphorization in the EAF process**
Minjoo Lee (Hanyang University, Korea)

# Development of hydrogen embrittlement resistant high-strength steel based on deep hydrogen trap design

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## Abstract

Under the background of carbon peaking and carbon neutralization, there is an increasing demand for advanced hydrogen embrittlement (HE) resistant high strength steels and novel mitigation methods. Among the proposed approaches, deep hydrogen trap design is a promising method that enable synergistically improve the HE resistance and strength/ductility. This report briefly reviews the discovery and recognition of hydrogen traps in steels, introduces the new methods in mapping hydrogen traps in metals, and summarizes the mainstream ideas of hydrogen trap regulation in steel. Furthermore, taking the HE resistant pipeline steels and ultra-high strength hot stamping steels as examples, the new progresses in the design and fabrication of second phases-induced deep hydrogen traps, such as inclusions and precipitates are described in detail. Finally, based on the above contents, the future research directions of deep hydrogen trap design in high-strength steels are prospected.

*Keywords: hydrogen embrittlement; high-strength steel; hydrogen trap; hydrogen diffusion.*

# The Use of Secondary Resources in Steel Manufacturing

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## Abstract

The steel industry is one of the largest energy consumers in the manufacturing sector, accounting for almost 6% of the total energy consumption in manufacturing. Energy constitutes a significant portion of the cost of steel production, from 20% to 40% in some cases. About 50% of an integrated facility's energy input in steelmaking comes from coal, 35% from electricity, 5% from natural gas and 5% from other gasses. This indicates the strong dependency of steelmaking on coke with heavy carbon footprint including extraction from underground coal mining, transportation and cooking process which produces a significant amount of greenhouse gas emissions. Reduced coke and energy consumption in steelmaking is crucial to ensure the competitiveness of the industry and to minimise environmental impacts, such as greenhouse gas emissions. Carbon neutral secondary resources such as those found in specific waste biomass or polymers can potentially be used in an economically viable and safe way to provide hydrogen and carbon to steelmaking processes and replace some or all the high-emissions coke source. This presentation details polymer injection technology (PIT) developed in SMaRT Centre @ UNSW which has been implemented by commercial EAF steelmakers in Australia, Asia and Europe, resulting in saving energy through reduction in electrical consumption, enhancement of furnace efficiency through improvement of slag foaming, yield increase, decease in coke consumption and diverting millions of waste tyres from landfill into manufacturing.

*Keywords: Carbon emission, EAF, carbon neutral resources, sustainability*

# Effect of ratio of scrap to iron source on slag-metal reactions in smelting and reduction process of iron ore

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## Abstract

With the depletion of high-grade iron ore and increase in the amount of steel scrap, a new ironmaking process utilizing both low-grade iron ore and/or steel scrap is required. The blast furnace and packed bed type partial smelting reduction process (PSR) are the most prospective reactors. However, steel scraps recovered from society are usually contaminated with tramp elements such as Cu, Sn, Ni, Cr. Therefore, the hot metal composition should be controlled considering the coexistence of tramp elements. Because FeO and MnO in the slag are reduced with Si and C in hot metal at the bottom of blast furnace, the hot metal composition will change in the direction of the equilibrium of the slag-metal reactions. The hot metal composition in the PSR is expected to change in a similar manner because the main raw materials are the same as those in the blast furnace. Because the PSR is a batch process, the operation is considered more flexible than that of the blast furnace. Accordingly, the temperature and partial pressure of oxygen at the bottom of the PSR furnace can be controlled over a wide range. In this work, an analytical model was developed to simulate the equilibrium of the slag–metal reaction at the bottom of such reactors. The effect of scrap ratio (iron mass ratio of scrap to scrap and sinter) on hot metal and molten slag compositions was thermodynamically analysed. and the optimal composition of hot metal under controlled temperature and oxygen potential was discussed.

*Keywords: ironmaking, thermodynamics, slag-metal reactions, steel scrap.*

# Effect of gangue oxide in HBI on dephosphorization in the EAF process

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**Abstract**

In order to reduce $CO_2$ emissions, steel companies are trying to develop the EAF steelmaking process instead of BF(–BOF) integrated route by employing high amounts of DRI/HBI. DRI/HBI as a substitute for virgin scrap in EAF have been used because DRI/HBI does not have tramp elements. Unfortunately, however, commercially available DRI contains a relatively high level of phosphorus, which adversely affects the properties of steels. The melting and dephosphorization behavior in EAF process conditions employing the 100% DRI/HBI have been less frequently investigated. Hence, we observed the morphology and distribution of elements with gangue oxides in commercially available HBI samples and investigated the melting phenomena of HBI as an alternative iron source during continuous heating using a high-frequency induction furnace.

Main composition of gangue oxides in HBI sample was $SiO_2$, $Al_2O_3$, and CaO in conjugation with unreduced iron oxide. Various size distribution of $SiO_2$-($Al_2O_3$-CaO) particles were observed in reduced iron matrix as well as in unreduced iron oxide phase.

Small amount of siliceous slag was formed when HBI was melted, thus, phosphorus content in steel was not varied during the melting stage. This is possibly due to the formation of relatively acidic slag. Using a FactSage calculation, the distribution ratio of phosphorus increases by adding CaO up to about 50% beyond which the melting point of slag is over 1500 ºC. So, the optimization of CaO content in the slag is required not only for maximum dephosphorization efficiency with good foamability but also for minimum slag volume with less refractory corrosion.

*Keywords: Hot briquetted iron (HBI), Gangue oxide, Melting, Slag foaming*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 4

November 21

10:50-12:30

# Technical **Oral Session _ Session 4**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 4 (A4)** **10:50 - 12:15, Nov. 21**

**Chair :** Hao Chen (Tsinghua University) Halla Hall A, 3F

10:50-11:20 **K-A0164** **[Keynote] Microalloyed cold-rolled advanced high strength steels**
Dong-Woo Suh (Pohang University of Science and Technology, Korea)

11:20-11:40 **I-A0485** **[Invited] Designing microstructures in low carbon microalloyed steels**
Arnab Chakraborty (The University of New South Wales, Australia)

11:40-12:00 **I-A0500** **[Invited] Ultra-high strength hot-forged lightweight steels**
Seok Su Sohn (Korea University, Korea)

12:00-12:15 **O-A0187** **Processing-microstructure-property relationship in governing high strength-high ductility combination in Fe-4Mn-4Ni-3Al-0.1C steel**
Linfeng Zhang (Hiroshima University, Japan)

# Microalloyed cold-rolled advanced high strength steels

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## Abstract

The incorporation of microalloying elements has played a significant role in the successful development of advanced high-strength steels. These elements are known to contribute to grain size refinement, fine carbide precipitation, and recrystallization retardation, resulting in enhanced strength and acceptable ductility in low carbon steels. Many studies have investigated the effects of microalloying elements, such as Nb, with a focus on the interaction between solute atoms or carbide precipitates and austenite recrystallization during hot deformation.

In the context of cold-rolled steels, microalloying elements are believed to participate in the recrystallization of cold-rolled ferrite, the reverse transformation into austenite upon heating, and the decomposition of austenite into various microstructural constituents during cooling, differentiating their role from that in hot-rolled steels. In this presentation, we aim to showcase recent advancements regarding the influences of microalloying elements on microstructural evolution in relation to heat treatment and the resulting tensile properties of cold-rolled steel. Particular emphasis is placed on the connection between processing conditions and microstructure evolution during annealing in Nb-Ti added steel, offering valuable insights to further our comprehension of their function in low carbon cold-rolled steels.

*Keywords: AHSS, microalloying, microstructure, cold-rolling, annealing.*

# Designing microstructures in low carbon microalloyed steels

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## Abstract

Low Carbon, Molybdenum-based microalloyed steels with polygonal ferrite microstructure are often used as structural components in the automotive industry due to their excellent stretch-formability. However, ferrite being softer phase requires advanced thermomechanical processing (a-TMP) microstructure engineering to enhance its yield strength via grain refinement. Additionally, harder martensitic microstructures obtained from same steel can become an attractive option for high strength applications following appropriate hardening and tempering treatments. While martensitic hierarchical evolution is understood for high Carbon microalloyed steels, it remains mostly unexplored for lower Carbon grades. Thus, two model microalloyed steels (Nb and NbMo steel) with compositions of C (0.1 wt.%), Nb (0.05 wt.%), and Mo (0 and 0.23 wt.%) were designed and subjected to optimized a-TMP targeting: (i) improve ferrite yield strength and (ii) study lath martensite evolution upon direct quenching. The engineered ferrite microstructure following two-phase ($\gamma+\alpha$) finish rolling at 750°C. resulted in finer polygonal ferrite grain sizes (~1.6 μm), and nanoprecipitation (~1.9 nm) leading to ferrite yield strength of (484 MPa) with ultimate tensile strengths >700 MPa for the NbMo steel. The NbMo steel strikingly exhibited coarser martensite hierarchical units than the Nb steel. Additionally, the NbMo steel showed lath substructures of intra-lath carbide-dislocation entanglements, without any twinning. However, the Nb steel exhibited dislocation networks, finer auto-tempered carbides along with long and short twins. Site-specific atom probe microscopy revealed variations in the C concentration of auto-tempered carbides for both steels. This highlights microstructural design capabilities in low C, Mo based microalloyed steels aimed at satisfying industrial demands for advanced properties.

*Keywords: Microalloyed steel, alloy design, thermomechanical processing, ferrite, lath martensite*

# Ultra-high strength hot-forged lightweight steels

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## Abstract

The demand for lightweight yet high-strength materials across various industries has stimulated the advancement of innovative steels with exceptional strength-to-weight ratios. Most of the reported ultra-high strength lightweight steels to date have been fabricated through cold rolling, followed by partial or complete recrystallization, thereby enhancing mechanical properties predominantly based on ultrafine-grained structures. In this study, we introduce a novel approach involving the development of an ultra-high strength hot-forged lightweight steel, which holds promise for potential applications in the automotive and aerospace sectors. The steel specimens were meticulously designed by incorporating low-density aluminum (Al) as the primary alloying element, along with microalloying elements vanadium (V), niobium (Nb), and boron (B). Following hot-forging, the steel specimens underwent a sequence of annealing and tempering processes to induce austenite reversion and precipitation hardening. The experimental results revealed remarkable strength levels, with yield strengths exceeding 1300 MPa and ultimate tensile strengths surpassing 1500 MPa. Furthermore, the steels exhibited moderate ductility ranging from 11% to 18%, thereby ensuring their suitability for demanding applications. The study further investigated the influence of processing parameters, such as annealing and tempering temperature, on the resulting microstructure and mechanical properties. The findings establish the successful development of ultra-high strength hot-forged lightweight steels, characterized by a unique combination of strength and ductility. The outcomes underscore the substantial potential of these steels for lightweight structural applications, presenting significant opportunities for weight reduction and enhanced fuel efficiency in transportation systems.

*Keywords: Lightweight steels; martensite; retained austenite; mechanical properties; tempering*

# Processing-microstructure-property relationship in governing high strength-high ductility combination in Fe-4Mn-4Ni-3Al-0.1C steel

**Linfeng Zhang**[1], Kazuhiro Matsugi[2], Zhefeng Xu[3],
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## Abstract

Breaking trade-off relationship between strength and ductility in steels has been a perpetual topic, since researchers have been pursuing more energy and resource-efficient manner to use steels. In this study, rolling, tempering and inter-critical annealing were innovatively combined to obtain high strength- high ductility combination in Fe-4Mn-4Ni-3Al-0.1C steel. The process referred as multi-step inter-critical annealing (MIA) was designed to accomplish the following objectives: (a) a stretched lamellar-shaped grain structure resulting from rolling at non-recrystallization region of austenite, (b) Mn/C-heterogeneous austenite inherited from carbides formed during tempering. Therein, Mn-depleted austenite areas originated from ferrite; meanwhile, Mn-enriched austenite areas originated from the carbide dissolution, (c) transformation hardening of Mn/C-depleted austenite area during cooling in the inter-critical annealing, (d) stress relaxation of Mn-enriched austenite area retained as retained austenite at room temperature. The obtained microstructure is composed of alternating lamellae of bainite and a special reverted structure on microscale, with the latter consisting of fresh martensite and retained austenite films on nanoscale. The yield strength and tensile strength of steel were increased from ~858 MPa and ~1267 MPa in direct inter-critical annealing process (DIA) to ~953 MPa and~ 1286 MPa in MIA respectively; total elongation was increased from 12% in DIA to ~27% in MIA. The modified Crussard-Jaoul analyses were used to evaluate the deformation behaviour of the steels. Due to lots of bainite formation, a relatively high initial strain hardening exponent (0.72 $m^{-1}$) was observed for the DIA steels. While lower initial strain hardening rate (0.32 $m^{-1}$) and more stages of work hardening because of increasing stable austenite and fresh martensite in the MIA steels ensured the excellent strength–ductility combinations.

*Keywords: strength-ductility paradox, inter-critical annealing, work hardening, Mn/C-heterogeneous austenite, tempering*

# Technical **Oral Session _ Session 4**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 4 (B4)** **10:50 - 12:25, Nov. 21**

**Chair :** Tomohiro Takaki (Kyoto Institute of Technology) 301, 3F
Da Seul Shin (Korea Institute of Materials Science)

10:50-11:20 **K-B0436** **[Keynote] High-performance phase-field lattice Boltzmann simulation of dendrite fragmentation and semisolid deformation during alloy solidification**
Tomohiro Takaki (Kyoto Institute of Technology, Japan)

11:20-11:40 **I-B0668** **[Invited] Effect of electric current on microstructural change of pure aluminum according to cavity shape**
Moon Jo Kim (Korea Institute of Industrial Technology, Korea)

11:40-11:55 **O-B0344** **Electropulsing treatment induced ultrafast precipitation and grain boundary migration**
Yuanshen Qi (Guangdong Technion-Israel Institute of Technology, China)

11:55-12:10 **O-B0338** **Fabrication of an anisotropic magnet by solidifying a semisolid slurry with electromagnetic vibration processing**
Mingjun Li (National Institute of Advanced Industrial Science and Technology (AIST), Japan)

12:10-12:25 **O-B0131** **In-situ Observation of Crack Formation in Semi-solid Copper Alloys**
Kohei Komori (Kobe Steel, Ltd., Japan)

# High-performance phase-field lattice Boltzmann simulation of dendrite fragmentation and semisolid deformation during alloy solidification

**Tomohiro Takaki**[1]

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## Abstract

Generally, in alloy casting, flows in the liquid region and mushy zone are caused by natural convection, forced flows, and solidification shrinkage. Notably, solute and isolated solid grain transport owing to such liquid flows is crucial for the formation of solidification microstructures and defects. One interesting and important solidification phenomenon caused by liquid flows during alloy casting is dendrite fragmentation, in which dendrite arms detach from the trunk. However, the detailed mechanism underlying dendrite fragmentation due to liquid flows is yet to be clarified. Moreover, when an external force is applied to a solid–liquid coexisting region, characteristic deformation behaviors, which are not observed in perfect solids and liquids, are known to occur. Such deformations, referred to as semisolid deformations, are characterized by solid–solid interactions and differing motions between liquid and solid grains. Because direct observations of liquid flows within metallic alloys are generally quite difficult, numerical simulations are essential to clarify the role of liquid flows in the solidification phenomenon.

In this study, we developed a polycrystalline solidification model by coupling the phase-field and lattice Boltzmann (PF–LB) methods, and the superior performance of this method could be attributed to parallel computing using multiple graphics processing units (GPUs). The developed model was applied to semisolid deformation. Moreover, we implemented adaptive mesh refinement for parallel computing with multiple GPUs in the PF–LB method, hoping to clarify the dendrite fragmentation mechanism caused by liquid flows. In this talk, I will describe our recent high-performance PF–LB simulations for dendrite fragmentation and semisolid deformation during alloy solidification.

*Keywords: Phase-field lattice Boltzmann method, High-performance computing, semisolid deformation, dendrite fragmentation, solidification.*

# Effect of electric current on microstructural change of pure aluminum according to cavity shape

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## Abstract

Grain refinement is one of powerful technique to enhance the strength and ductility of metallic materials. Recently, electrically-assisted solidification is being studied as an alternative method to refine the microstructure of metallic materials. It has been reported that grain can be effectively refined by applying electric current to the liquid metal during solidification. Here, effect of electric current on grain refinement of pure aluminum according to cavity shape was investigated based on experimental and numerical approaches. Three cavity shapes were prepared: cylinder, cube and cuboid with similar cavity volumes. Although the cooling behavior of liquid aluminum in three cavity shape was different due to the difference in cavity shape, grain refinement was clearly observed with a similar grain sizes in all three types of cavity shape under the same electrical condition. Based on numerical simulation, it was confirmed that the circulating flow of liquid aluminum with a shear rate strong enough to cause dendrite fragmentation was formed by applying electric current. The circulating flow is also expected to affect the final shape of refined zone by delivering the nuclei to unsolidified region. This work can contribute to examine the effectiveness of electrically-assisted solidification in a real product with a complex shape.

*Keywords: Aluminum, Grain refinement, Electric current, Microstructure, Numerical simulation*

# Electropulsing treatment induced ultrafast precipitation and grain boundary migration

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## Abstract

Using periodic electric current pulses, i.e., electropulses, to stimulate microstructure evolution such as recovery and recrystallization after cold/warm working , and precipitate formation and dissolution after solution-treatment, has been drawing increasing attention. The pulsed electric current scattering on the crystal lattice defects including dislocations, grain boundaries, and heterophase interfaces could trigger unique phenomenon that cannot be achieved by traditional heating. Therefore, electropulsing (EP) treatment as a novel post-thermomechanical processing technique possesses the potential to surpass the conventional annealing and aging techniques with respect to energy saving and property enhancement, and provide unique microstructure design strategy. In this talk, I will present our recent results on EP induced ultrafast precipitation and grain boundary migration phenomenon.

*Keywords: Electropulsing treatment; precipitation; grain boundary migration; electron microscopy.*

# Fabrication of an anisotropic magnet by solidifying a semisolid slurry with electromagnetic vibration processing

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## Abstract

An anisotropic $Nd_2Fe_{14}B$ magnet has been applied widely because of a high maximum energy product. To fabricate such a magnet, two main techniques have been developed. One is powder metallurgy and the other is hot deformation or hot press of fine ribbons using an upsetting die. In the present work, we reported on a novel technique, by which a bulk anisotropic magnet can be produced by solidifying the $Nd_{70}Cu_{30}$–50wt% $Nd_2Fe_{14}B$ alloy from the semisolid state when electromagnetic vibration (EMV) was imposed.

The as-cast ingot was set in a static magnetic field and heated to the semisolid state. Alternating current was imposed to flow through the ingot to yield the Lorentz force according to Fleming left hand rule. The periodic switchover of the force direction drove the specimen to vibrate centering the equilibrium position, and thus EMV was produced.

The EMV imposed at a low frequency was effective in segmenting the developed long $Nd_2Fe_{14}B$ phase into fine short platelets and that at a high frequency was effective in aligning the segmented platelets with their *c*-axes parallel to the direction of the magnetic field. Electron backscatter diffraction (EBSD) patterns and the magnetic properties measured by a vibrating sample magnetometer (VSM) confirmed the anisotropy of the specimen solidified by the two-step EMV processing. The segmentation mechanism was discussed and the alignment driving forces were considered, revealing that both the magnetic field and electromagnetic forces are important in orienting the $Nd_2Fe_{14}B$ platelets in the semisolid slurry.

*Keywords: Anisotropic magnet; $Nd_2Fe_{14}B$ phase; Semisolid; Solidification; Electromagnetic vibration*

# In-situ Observation of Crack Formation in Semi-solid Copper Alloys

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## Abstract

The development of technologies to reduce environmental impact is an urgent issue for achieving carbon neutrality by 2050. In this context, there is a particular need to improve the performance of electrification and communication technologies, such as EVs, AI, and IoT. Because of their high electrical conductivity, copper alloys are especially used in electrical devices for these applications, and the development of compositional design and microstructure control technologies is being pursued intensively. In the development of such alloys, it is essential to reduce defects in the manufacturing process. Solidification cracking during casting is difficult to reduce in the later processes, so there is a need to elucidate the formation mechanism and develop technologies to reduce such cracking.

In-situ observation of solidification by time-resolved X-ray imaging is a suitable observation method to empirically understand the solidification process. So far, the formation process of casting defects by shearing and deforming semi-solid steels and aluminium alloys has been reported. In this study, we observed the deformation behaviour of Cu-Fe-P alloys under shear stress while holding them in the semi-solid state to clarify the characteristics of the crack formation mechanism in copper alloys. Several alloys of Cu-0.1mass%Fe containing P in the range of 0.03mass% to 0.15mass% were used for the observation. As a result, it was observed that cracking is dependent on P concentration, and when P concentration is high, the melting point of grain boundary is locally lowered because of P concentration, the liquid film is formed, and cracks occur starting from there.

*Keywords: Copper alloy, Time-resolved and in-situ observation, X-ray imaging, Crack formation*

# Technical **Oral Session _ Session 4**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 4 (C4)** **10:50 - 12:25, Nov. 21**

Chair : Dong Ik Kim (Korea Institute of Science and Technology) 201A, 2F
Guoqing ZHANG (AECC Beijing Institute of Aeronautical Materials)

10:50-11:20 **K-C0478** **[Keynote] Exploring the Insight into the Microstructure-Mechanical Property Relationship of Additive Manufactured Ni-Based Superalloys**
Hyun-Uk Hong (Changwon National University, Korea)

11:20-11:40 **I-C0422** **[Invited] Development of γ′-strengthened CoNi-base powder superalloys suitable for additive manufacturing**
Longfei LI (University of Science and Technology Beijing, China)

11:40-11:55 **O-C1032** **Micro-alloying enhances creep resistance of additively manufactured IN718 alloy**
Li Gong (Tsinghua University, China)

11:55-12:10 **O-C0081** **Influence of solution treatment on the γ' phase precipitation behavior in K444 cast nickel-based superalloy**
Y.s. Xie (Harbin Engineering University, China)

12:10-12:25 **O-C0815** **Precipitation Mechanism of η-Ni3Ti Phase and Its Inhibition Method by Hf Microalloying in a Nickel-based Superalloy with High Ti/Al Ratio**
Meiqiong Ou (Institute Of Metal Research, Chinese Academy Of Sciences, China)

# Exploring the Insight into the Microstructure-Mechanical Property Relationship of Additive Manufactured Ni-Based Superalloys

**H.-U. Hong[1]**, C.H. Yang[1], C.H. Lee[1], J. Lee[2], S.-Y. Jun[3], P. Lours[4], B.H. Lee[5], J.H. Jang[6], B.S. Lee[7], H.J. Lee[7]

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## Abstract

In recent years, there has been growing exploration of new processing and fabrication routes for superalloys using additive manufacturing (AM) techniques, such as laser and electron beam melting technologies. Microstructures and tensile/creep properties were characterized for as-fabricated and heat-treated SLMed Inconel 625 and 939W samples. Various heat treatments, including the formation of serrated grain boundaries, were extensively designed to have optimal microstructures. It is interesting that different SLM conditions (recommended by each printer company) make a similar microstructure evolution, but different microstructure features can be found in nano-scale (e.g. columnar width, nano-sized MC carbides, and oxides). Recently, we developed a new high γ′ superalloy suitable for AM by using thermodynamic calculations. The design approach intended to increase AM processability while maintaining the high-temperature strength of the reference superalloy René 80. Using the conventional René 80 composition as a baseline, Ti reduction (5→3 wt.%), 2.5 wt.% Ta addition, and 1.0 wt.% Hf addition successfully prevented crack formation after EBM fabrication and considerably improved the characteristics of alloy powders, which exhibited more spherical shapes with fewer satellites. Atom probe tomography results indicated that the partitioning of Ti, Al, and Ta atoms into the γ′ phase facilitated to increase in the lattice misfit at the γ/γ′ interface, ad made it more difficult for dislocations to cut through γ′ particles. The tensile/creep properties of AMed superalloys will be discussed with respect to their typical compositions and microstructures.

*Keywords: Superalloys; Additive manufacturing; Microstructure; Heat treatment; Creep*

# Development of γ′-strengthened CoNi-base powder superalloys suitable for additive manufacturing

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**Abstract**

As a promising advanced high-temperature material, γ′-strengthened Co-base superalloy has attracted more and more attention since 2006 and has been continuously developed to the multicomponent CoNi-based superalloys with better comprehensive properties in the past decade. However, most researches focus on CoNi-based cast or wrought superalloys and only a few of work on CoNi-based powder superalloys, which are more suitable for manufacturing complex shaped parts by traditional powder metallurgy (PM) or modern additive manufacturing (AM). In this work, γ′-strengthened CoNi-base powder superalloy is developed based on our previous Materials Genome Engineering (MGE) approach, with focusing on the weldability. The microstructures and mechanical properties of this alloy which is prepared by vacuum induction melting and argon gas atomization (AA) were investigated under different routes, i.e., directly by hot isostatic pressing (HIP) process or By AM process plus HIP process. The results indicated that the developed CoNi-based powder superalloys are suitable for additive manufacturing, either by electron beam melting (EBM) or by selective laser melting (SLM). Through optimizing processing parameters, the as-built alloy which has no inner crack with the porosity of <0.15% is composed of epitaxially grown columnar grains with a strong <001> texture. HIP process can further decrease the porosity of the as-built alloy, but do not change the as-built microstructure significantly. Meanwhile, the as-HIPed microstructure is composed of equiaxed grains with the porosity of <0.1%. Both the alloys by AM+HIP or HIP demonstrate good mechanical properties, showing the good industrial application potential.

*Keywords: γ'-strengthened CoNi-base powder superalloy, electron beam melting, hot isostatic pressing, microstructure, mechanical properties.*

# Influence of solution treatment on the γ' phase precipitation behavior in K444 cast nickel-based superalloy

**Youshui Xie[1],** Xiaopeng Li[1], Renheng Han[1], Yihan Zhao[1] , Yulong Liang[2], Chengzhi Zhao[1], Hexin Zhang[1]

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## Abstract

The morphology and size of the γ' phase play a significant role in the fabrication of superalloy and the properties under severe conditions. The evolution of the size, morphology and distribution of γ' phase with holding time and solution temperature are discussed in detail and systematically in the present investigation. The γ' phase acquired after heat treatment exhibits a variety of morphologies, consisting of irregularly coarse primary γ' phase along the grain boundaries, cubical secondary γ' phase homogeneously distributed on the matrix, and fine spherical tertiary γ' phase in γ matrix channel. With the increase of solution temperature from 1130°C to 1190°C, the size of secondary γ' phase gradually increases, while the size of tertiary γ' phase reaches the minimum value at 1160°C. At 1160°C, gradually the size of the secondary γ' phase increases as the solution time increases from 1.5h to 5.5h, while the size of the tertiary γ' phase reaches the minimum value 46.92nm at 3.5h holding time. In addition, the precipitation behavior of the tertiary γ' phase precipitated in the γ channel during aging is consistent with that of the γ' phase precipitated during solution cooling. This research helps to understand the evolutionary behavior of the γ' phase in nickel-based superalloy during heat treatment and provides a fundamental theory for the optimization of the heat treatment of K444 alloy.

*Keywords: Nickel-based superalloy, Precipitation behavior, Microstructure, γ' phase,Size.*

# Precipitation Mechanism of η-$Ni_3Ti$ Phase and Its Inhibition Method by Hf Microalloying in a Nickel-based Superalloy with High Ti/Al Ratio

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## Abstract

Nickel-based superalloys with high Ti/Al ratio are commonly suffering to the precipitation of undesirable η-$Ni_3Ti$ phase during long-term thermal exposure. This study has firstly investigated the precipitation mechanism of η phase in K4750 alloy (Ti/Al=2.5). The orientation relationship between η/γ is clarified as $<11\bar{2}0>_\eta//<1\bar{1}0>_\gamma$, $\{0001\}_\eta//\{111\}_\gamma$ and twelve η phase variants with an misorientation of 70.5° of each other can be observed. The $\{0001\}_\eta//\{111\}_\gamma$ interface marked as A-type is coherent, the $\{11\bar{2}0\}_\eta//\{1\bar{1}0\}_\gamma$ marked B-type is incoherent, and the preferential growth of the high-energy B interface will induce a thin-plate morphology of η phase. It is found that the metastable extra-large γ′ (EL-γ′) plays a role in all the solid-state phase transformation reactions involved with the precipitation of intragranular η phase, including produced by MC decomposition, induced by $M_{23}C_6$ precipitation and absorbing γ′ phase. The composition of EL-γ′ and η phases was similar, but the stability of EL-γ′ is lower than η phase (the calculated formation energies of $L1_2$-$Ni_3Ti$ and $D0_{24}$-$Ni_3Ti$ are -0.4684 and -0.4863 eV/atom, respectively), which is the thermodynamic driving force for EL-γ′→η. Their structure difference can be attributed to the arrangement order of the close-packed planes and could be smoothed out through stacking faults, which is the kinetic mechanism that the intermediate step EL-γ′→η is prone to occur. Based on above, we have secondly conducted Hf microalloying method. It is found that Hf enters into MC and γ′ phases and enhances their stability, thereby delaying the precipitation of η phase, and thus increasing the stress rupture life after thermal exposure.

*Keywords: Nickel-based superalloys; Long-term thermal exposure; Solid phase transition; η phase; Hf microalloying*

# Technical **Oral Session _ Session 4**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 4 (D4)** **10:50 - 12:40, Nov. 21**

**Chair :** Chair:Shinji Kumai ( Tokyo Institute of Technology), Soong-Keun Hyun (Inha University) Samda Hall A, 3F

10:50-11:20 **K-D0381** **[Keynote] Aluminium upgrade recycling for carbon neutrality**
Shinji Kumai (Tokyo Institute of Technology, Japan)

11:20-11:35 **O-D0013** **Study on determination method of rare earth elements in aluminum alloy**
Zhang Jie (Iron & Steel Research Institute of Ansteel Group, China)

11:35-11:55 **I-D0335** **[Invited] Improvement of battery performance by applying iron-containing recycled aluminium to current collector-free anode of lithium-ion batteries**
Shoichi Hirosawa (Yokohama National University, Japan)

11:55-12:10 **O-D0008** **Dual heterogeneous precipitates promoting an excellent high-temperature strength-ductility synergy in TiB2/Al-4.5Cu composites via multi-trace alloying strategy and dynamic permeability molten salt approach**
Yanqing Xue (Xi'an University of Posts and Telecommunications, China)

12:10-12:25 **O-D0066** **Simultaneous improvement of strength and ductility aluminum matrix composites containing sub-micron high-entropy alloy (HEA) particles**
Chahee Jung (Kookmin University, Korea)

12:25-12:40 **O-D0592** **Thermal Stability and Mechanical Response in Segregation-Engineered Nanocrystalline Al-TM-RE Alloys: A Combinatorial Study**
Jungho Shin (Gangneung-Wonju National University, Korea)

# Aluminium upgrade recycling for carbon neutrality

**Shinji Kumai**[1]

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## Abstract

Aluminium's lightness helps to reduce $CO_2$ and other greenhouse gas (GHG) emissions during transportation by vehicles, and its high recyclability will undoubtedly contribute to the realization of carbon neutrality. However, the need for GHG reduction is not limited to the phase of product use; what is important is reducing GHGs emitted throughout an individual product's lifecycle (LC-GHG). The production process of an aluminium virgin ingot uses a large amount of electricity and, depending on the electricity source, emits large amounts of GHGs. However, because of the low melting point of aluminium, the GHG emission rate for the fabrication of recycled ingots from used scrap is extremely low. The environmental impact of aluminium can be greatly reduced through recycling. However, recycled aluminium ingots are currently used for the fabrication of lower-grade materials (i.e., cascade recycling) and cannot be used for the production of high-purity and high-grade wrought materials, for which demand is expected to increase in the future. Researching and developing upgrade recycling methods for aluminium is therefore urgently needed, where recycled ingots with a lower environmental impact are used for the fabrication of wrought materials. This approach will substantially reduce GHG emissions and ultimately promote a sophisticated resource-recycling society in which aluminium resources can be almost completely recycled. Currently, Japan does not smelt aluminium domestically; it imports all virgin ingots from overseas. Establishing an advanced recycling and utilization system for aluminium scrap is also important to ameliorate this dependency on foreign countries for virgin ingots used for wrought applications.

*Keywords: aluminium, carbon neutrality, greenhouse gas emission, lifecycle assessment, upgrade recycling.*

# Study on determination method of rare earth elements in aluminum alloy

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## Abstract

Analysis of light rare earth elements(REEs) La, Ce, Pr, Nd, Sm by inductively coupled plasma atomic emit spectrometry(ICP-AES), meantime, using orthogonal design of the experimental apparatus has been optimized working conditions. In the experimental wavelength, the REEs had measured the standard curve, and the correlation coefficient of the regression equation, the linear range of up to four orders of magnitude. The RSD of the samples parallel measurement is at 0.17%～2.58% , the recovery of the experiment result is 93.00%～110.00%, which express the sophistication and accurate of the experiment is good.

Due to the extensive application of REEs in various industries, the accurate analysis of REEs has always been a difficult and hot issues in the field of analytical chemistry[1].ICP-AES analysis is a rapid and accurate means for multi-element, but because of the rare earth elements spectrum interference serious, REEs coexist in a variety of circumstances analysis, often must be pre-separation[2-3], which led to a long cycle analysis, analysis errors. To overcome them, between the spectral interference by the matrix matching[4], correction factor[5-7], computer simulation[8]. This experiment used the *K* matrix method of chemometrics to handle the spectrum test data of the REEs in the actual sample[9-10].The aluminum alloy samples were corrected by the *K* matrix respectively.The mathematics model will overcome the mutually interference in the REEs. This experiment didn't carry on separation to the REEs, carried out the fast and accurate measurement of the REEs.

*Keywords: inductively coupled plasma atomic emission spectrometry(ICP-AES)； rare earth elements(REEs)； aluminum alloy； K matrix； interference correction.*

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# Improvement of battery performance by applying iron-containing recycled aluminium to current collector-free anode of lithium-ion batteries

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## Abstract

Lithium-ion batteries with graphite anode have been utilized in a condition close to the theoretical capacity of graphite, and thus the application of current collector-free aluminum anode has been attempted for further increase in capacity because theoretical capacity of aluminum is 2.7 times larger than that of graphite. In this study, Al-2mass%Fe alloy was applied as a noble anode material, and found to possess better discharge capacity retention and Coulomb efficiency than those of 4N-purity aluminum. Such improvement of battery performance in Al-2mass%Fe anode is attributed to the formation of more stable reaction layers of randomly oriented nanocrystalline AlLi owing to finely dispersed intermetallic compounds of $Al_6Fe$ and $Al_3Fe$. This result would expand application ranges of recycled aluminum containing larger amounts of impurity iron, with less future demand from foundry industries to be partly compensated.

*Keywords: Lithium-ion batteries, Aluminum anode, Aluminum alloys, Recycling, Nanocrystalline microstructure*

# Dual heterogeneous precipitates promoting an excellent high-temperature strength-ductility synergy in $TiB_2$/Al-4.5Cu composites via multi-trace alloying strategy and dynamic permeability molten salt approach

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## Abstract

High-temperature coarsening or even decomposition of θ'-$Al_2Cu$ precipitates is an intractable dilemma during the service of aluminum-copper based alloys and composites. Here we demonstrate a multi-trace alloying strategy of Mg, Mn, Ag and a multistep heat treatment process to stabilize the θ'-$Al_2Cu$ precipitates in $TiB_2$ particles reinforced aluminum-copper matrix composites fabricated by dynamic permeability molten salt approach. By generating thermostable T-$Al_{20}Cu_2Mn_3$ and Ω-$Al_2Cu$ precipitates, or stabilizing θ'-$Al_2Cu$, excellent heat resistance is acquired in the $TiB_2$/Al-Cu-Mn-Mg composites, exhibiting an ultrahigh strength (ultimate tensile strength, 264 ± 17.9 MPa) and ductility (15.6 ± 2.9%) even at 573K. Meanwhile, the multiple heterogeneous microstructures successfully induced a remarkable combination of strength (ultimate tensile strength, 612 ± 8.6 MPa) and ductility (18.1 ± 3.7%) at ambient temperature. It is evidenced that the thermostable precipitation hardening facilitated by geometrically necessary dislocations and dispersed homogeneous $TiB_2$ particles induced by the dynamic permeability molten salt approach were responsible for the well-performed mechanical properties. The result sheds light on simultaneously improving the strength and ductility of Al matrix composites and provides a new avenue to cast high-performance complex-shaped components.

*Keywords: Aluminium matrix composites (MMCs); Micro-alloying; Heat treatment; Aging behaviour; Microstructures; Mechanical properties*

# Simultaneous improvement of strength and ductility aluminum matrix composites containing sub-micron high-entropy alloy (HEA) particles

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## Abstract

Aluminum matrix composites (AMCs) have been extensively studied in future mobility industries because of their excellent mechanical properties and elastic modulus. Although materials containing carbon and ceramics are used as reinforcement for AMCs, they have a poor wettability with aluminum. To solve this, high entropy alloys (HEAs) have recently attracted a great deal of attention as reinforcement for aluminum matrix composites. They have high wettability with Al and high strength while maintaining the crystal structure.

In this study, AMCs reinforced by sub-micron $Al_{0.5}CoCrCuFeNi$ HEA particles were produced by powder metallurgical routes. First, HEA powder was produced by high-energy attrition milling. And then, they were subjected to a thermal plasma process to make them sub-micron. 2 vol% of HEAs was then attrition milled with Al powder. The composite powder was hot-rolled and was subjected to heat treatment for 12 h at 500 °C. Reinforcing effect of Al0.5CoCrCuFeNi HEA particles on the mechanical properties of AMCs will be discussed in the microstructural perspective.

*Keywords: Aluminum matrix composite, High-entropy alloy, Mechanical milling, Hot-rolling*

| O-D0592 |

# Thermal Stability and Mechanical Response in Segregation-Engineered Nanocrystalline Al-TM-RE Alloys: A Combinatorial Study

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**Abstract**

The deliberate use of solute enrichment at interfaces such as grain boundaries, otherwise known as segregation engineering, is a promising approach to tailor the properties of interface-dominated materials including nanocrystalline alloys. The ensuing chemical and structural evolution at grain boundaries can give rise to thermal stability and excellent mechanical properties, but the interplay between enrichment, phase decomposition, grain growth, and corresponding links to mechanical behavior exist in a vast composition and processing space. In this study, combinatorial synthesis and high-throughput approaches were applied to segregation-engineered nanocrystalline Al-(Ni, Fe, Mg)-(Ce, Y) alloys to assess the evolution of microstructure and resulting mechanical behavior as functions of alloying content and annealing conditions. In addition to the identification of alloys and processing space that gives rise to exceptional thermal stability, strength retention, and homogeneous plastic flow, we construct combined thermal stability and deformation mechanism maps that delineate several regimes of behavior. Such high-throughput materials screening exercises promise to accelerate the discovery of an optimized suite of properties in segregation-engineered nanocrystalline alloys, particularly in multi-component systems. A direct outcome of our alloy downselection exercise is presented in the fabrication of fully dense bulk nanocrystalline Al alloys with exceptional thermal stability via a powder metallurgy approach.

*Keywords: aluminum alloys, segregation engineering, grain boundary engineering, nanocrystalline alloys, combinatorial screening*

# Technical **Oral Session _ Session 4**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 4 (E4)** **10:50 - 12:50, Nov. 21**

**Chair :** Jung Gi Kim (Gyeongsang National University), Cecilie Funch (The University of Sydney) Halla Hall B, 3F

10:50-11:20 **K-E0818** **[Keynote] Unlocking the Potential of Selective Electron Beam Melting: Revolutionizing Additive Manufacturing and Expanding Material Possibilities**
Tang Huiping (Hangzhou City University, China)

11:20-11:40 **I-E0602** **[Invited] Micro-cracking Behaviors of Melt Pools Deposited by Additive Manufacturing Processes**
Yoon Suk Choi (Pusan National University, Korea)

11:40-12:00 **I-E0683** **[Invited] Crack-free eutectic high-entropy alloy claddings on ductile cast iron by extreme high speed laser cladding.**
Andrew Ang (Swinburne University of Technology, Australia)

12:00-12:15 **O-E0430** **Adapting Material Extrusion Control System for a 3D Food Printer**
Ichimori Izumi (Yamagata University, Japan)

12:15-12:30 **O-E0286** **3D Bioelectronic Printer for Nerve Regeneration**
Juyong Lee (Seoul National University, Korea)

12:30-12:50 **I-E1115** **[Invited] Nonlinear thermal distortion and its compensation of additively manufactured components via electron beam powder bed fusion**
Pan Wang (Singapore Institute of Manufacturing Technology, Singapore)

# Unlocking the Potential of Selective Electron Beam Melting: Revolutionizing Additive Manufacturing and Expanding Material Possibilities

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## Abstract

Selective Electron Beam Melting (SEBM) has emerged as a game-changing technology in additive manufacturing, reshaping the landscape of component fabrication. By offering unparalleled precision and exceptional material properties, SEBM has opened new frontiers to produce highly intricate and customized components. Overcoming the limitations of traditional manufacturing techniques, SEBM possesses a unique capability to fabricate complex geometries and intricate structures with remarkable ease.

Within the realm of materials, SEBM has garnered significant attention for its impact on microstructure, mechanical properties, and materials optimization strategies. Cutting-edge research demonstrates remarkable advancements achieved through SEBM, with notable improvements observed in density, strength, and overall structural integrity. The versatility and adaptability of SEBM are showcased through its application across a wide range of materials, including refractory alloys, composites, and lattice structures, unlocking diverse possibilities in various industries.

In the medical field, SEBM-fabricated devices hold tremendous promise, exemplified by tantalum bone implants and orthopedic structures. These SEBM-manufactured components exhibit exceptional biocompatibility, osseointegration, and the potential for patient-specific customization. Although challenges and opportunities exist in implementing SEBM within the medical domain, continued advancements in this technology pave the way for transformative breakthroughs in patient care.

The future prospects of SEBM involve integrating advanced computational modeling, material design, and process optimization techniques. These advancements unleash untapped potentials, further enhancing the capabilities and expanding the applications of SEBM. Through computational modeling, more accurate prediction and control of the fabrication process can be achieved, while optimized material design and process parameters enable the production of tailored components with increased efficiency.

*Keywords: Additive manufacturing, Selective electron beam melting, Microstructure, Metal and alloy, Medical applications*

# Micro-cracking Behaviors of Melt Pools Deposited by Additive Manufacturing Processes

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## Abstract

The micro-cracking behaviors of melt pools processed by different additive manufacturing techniques were experimentally and numerically investigated for the following cases: medium carbon steel melt pools deposited on gray cast iron using direct energy deposition (DED); TiAl melt pools deposited by the laser power bed fusion (PBF) process. In the first topic, single track and multi-layers of medium-carbon steel (AISI H13) powders were additively deposited on gray cast iron using DED. The crack formation mechanism was thoroughly investigated by checking the local chemistry variation and the resulting microstructural evolution upon exposure to thermal cycles during the DED process. The result indicated that cracks formed by an indirect exposure to multiple heating-cooling thermal cycles, not by a direct exposure to a melting-cooling (solidification) cycle. In the second topic, the crack formation mechanisms of Ti-48Al-2Cr-2Nb single tracks processed by PBF were extensively investigated in a wide range of laser powers and scan speeds. The crack patterns were categorized by their directionalities, and micro-cracking behaviors were characterized by combining the fractography and the microstructural analysis. Further, thermal-mechanical finite element method (FEM) simulations were performed to predict the distribution of temperatures and thermal stresses during the melt pool formation. On the basis of the combined results, the cracks formed in keyhole, transition, and conduction modes were clarified as a solidification crack and/or a thermal crack. In addition, the formation of these cracks was thoroughly understood in terms of thermal stresses and microstructural factors that affect the crack susceptibility. Finally, comprehensive mechanisms responsible for cracking of Ti-48Al-2Cr-2Nb single tracks were proposed for different PBF process conditions.

*Keywords: Melt pools, micro-cracking, additive manufacturing, cast iron, TiAl*

# Crack-free eutectic high-entropy alloy claddings on ductile cast iron by extreme high speed laser cladding.

Hank Lloyd [1], Ashok Meghwal [1], Christopher C. Berndt [1], **Andrew Siao Ming Ang** [1,*]

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## Abstract

High-entropy alloys (HEAs) are an emerging class of materials with distinctive structural properties that, realizing their potential as next-generation coating materials, provide protection against extreme wear and corrosive environments. In the present work, to investigate the use of HEAs as wear protection coatings on cast-iron-based mining components, Ni-rich eutectic HEA coatings were applied to ductile cast iron using extreme high speed laser cladding (EHLA). The HEA coatings were explored as an alternative to conventional Ni-rich refurbishment powders.

Near-dense and crack-free EHLA coatings were obtained. The EHLA process with ultra-low heat input resulted in a narrower cladding interface than achievable by conventional laser metal deposition. This resulted in a low ledeburite fraction, retained austenite, and martensitic shells around graphite nodules in the cast-iron substrate near the interface. The coating retained the eutectic phase composition (FCC + BCC/B2) of the original powder without any intermetallic formation. Microstructural analysis revealed a grain structure transition in response to processing parameters, producing 'feathered' columnar grains and plate structures that further transitioned to equiaxed gains towards the cladding surface. EBSD maps of the coating verified the eutectic nature of the coating with compositional segregation within different phase structures. Microhardness profiling was performed to investigate the hardness of the coating and hardness variation with respect to different phase structures was studied. The overall study demonstrated that HEA coatings produced using the EHLA process offer exciting prospects for the development of dense and crack-free coatings for challenging engineering environments.

## Keywords

High Entropy Alloys (HEAs); Extreme High Speed Laser Cladding (EHLA); Microstructure; Mechanical Properties.

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# Adapting Material Extrusion Control System for a 3D Food Printer

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**Abstract**

The screw-type 3D printer “NP-2500” can print foods using a variety of food inks, such as cookie dough and surimi. It is necessary to adjust printing parameters, for example extrusion volume and printing speed, depending on the physical properties of food inks. Additionally, the volume of extrusion and the suitable printing parameters depends on the hardware size (nozzle diameter) and the environment (temperature and humidity) at which the 3D food printer is placed.

After the printing and during printing, we have to visually review the 3D foods and how the food inks is extruded, in order to tune the parameters manually for preventing the under-extrusion or over-extrusion. Automatic monitoring for tuning the printing parameters is still a big challenge in 3D food printing systems.

In this study, we aim to develop a monitoring system to optimize the volume of food ink extrusion for 3D food printers during the printing process, referring to previous studies that performed in-situ monitoring system for FDM 3D printers.

*Keywords: 3D printer, 3D food printer, Additive manufacturing, real-time analysis*

# 3D Bioelectronic Printer for Nerve Regeneration

**Ju-Yong Lee[1]**, Jooik Jeon[2], Joo-Hyeon Park[3], Yea-Seul Park[4], Se-Hun Kang[5], Min-Sung Chae[6], Kang-Sik Lee[7], Jung Keun Hyun[8], Seung-Kyun Kang[9]

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## Abstract

The increasing clinical demands for customized conformal contact of electronics to a patient's lesion have brought about emerging technologies, driven by the needs of focused, continuous, and high-precision clinical treatment. Currently, two-dimensionally fabricated soft matter equipped with stretchable components can conformally wrap smooth surfaces, but they cannot support the types of complex structures such as hollow, branched, and tubular forms within a volumetrically limited space that bio systems possess. The challenges lie in the fact that structural deformation to adapt to the target shape after fabrication is bounded to continuous matter's elastic restriction, with limitations of fabrication form factor. While reverse-engineering based pre-designed structures provide good conformability, incorporation of electronics into the prearranged structure costs a lot. To overcome these challenges, we have developed voxelated electronic materials for 3D integrated circuitry and sensors within customized structures driven by multi-material printing. We implemented a stereographical circuit arrangement strategy with voxelated semiconductors guided by digitally programmed 3D integration circuits in customized structures. As a demonstrative example, we have printed a 3D customized electroceutical and conducted in-vivo experiments to prove the efficacy of this innovative technology. This advancement in 3D printing technology will pave the way for personalized, high-precision clinical treatment, and revolutionize the way we approach medical care.

*Keywords: 3D bioelectronics, Biodegradable electronics, Multi-material printing, 3D Active components, Wireless neuro-stimulator*

# Nonlinear thermal distortion and its compensation of additively manufactured components via electron beam powder bed fusion

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## Abstract

Electron beam powder bed fusion (EB-PBF) utilizes a high-energy electron beam to process the metallic powders under a vacuum atmosphere. Taking advantage of its high preheating temperature capacity of up to 1200 ºC, EB-PBF facilitates in situ stress release to benefit complex geometrical components fabrication. However, the thermal gradient between the last build layer and the first build layer results in a differential shrinkage during its cooling step. The conventional approach of applying globally uniform scaling factors to compensate for part shrinkage is insufficient and introduces dimensional errors of EB-PBF components. To address this, we analyse distortion patterns in each global direction (X, Y, Z) and reveals distinct thermal distortion rules. Leveraging this insight, our in-house MatLab script uses experimentally measured localized nonlinear correction formula as input to generate a compensated STL file as the output. Through a case study involving the compensation of a large-scale bracket (320 mm long), we validate our approach's effectiveness in mitigating shrinkage accumulations across all coordinate directions within 0.15 mm. This pioneering digital compensation method sets a foundation for enhancing the precision and quality of EB-PBF components, thereby accelerating the industrial adoption of EB-PBF technology.

*Keywords: Electron beam melting; Digitalization; Thermal distortion; Dimensional compensation; Industrial application*

# Technical **Oral Session _ Session 4**

## **Symposium F :** Thin Films and Surface Engineering

### Thin Films and Surface Engineering 4 (F4) 10:50 - 12:30, Nov. 21

Chair : Nan Li (Los Alamos National Laboratory), Surinder Singh (Swinburne University of Technology) 202A, 2F

10:50-11:20 **K-F1120** **[Keynote] Organic – Inorganic Metal Halide Materials for Photovoltaics**
Hyunjung Shin (Sungkyunkwan University, Korea)

11:20-11:40 **I-F0891** **[Invited] High-entropy alloy films: a review**
Qing Wang (Dalian University of Technology, China)

11:40-12:00 **I-F0360** **[Invited] Enhancement of coercivity for Sm(Fe-Co)-based thin films through the infiltration of the elements**
Toshiyuki SHIMA (Tohoku Gakuin University, Japan)

12:00-12:15 **O-F0020** **Effects of Surface Modification on Primary Water Stress Corrosion Cracking Initiation Behaviour of Nickel-based Alloy**
Seunghyun Kim (Korea Institute of Materials Science, Korea)

12:15-12:30 **O-F0893** **Fuzz evolution of NbMoTaW series multi-principal element alloy films by high-flux He ions irradiation**
Xianxiu Mei (Dalian University of Technology, China)

# Organic – Inorganic Metal Halide Materials for Photovoltaics

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## Abstract

Power conversion efficiency (PCE) of Perovskite solar cells (PSCs) is over 25.7%. Despite PSCs' high PCEs, their operational as well as environmental instability remains to be solved and restrict PSCs' commercialization. Currently, the state-of-the-art PSC is used almost pure a-$FAPbI_3$ (Formamidinium lead tri-iodide) as an absorber and 2,2',7,7'-tetrakis[N,N-di(4-methoxyphenyl)amino]-9,9'-spirobifluorene (Spiro-OMeTAD) as hole transporting layer (HTL) in the *n-i-p* normal structure of PSCs. A chemical-deriven phase transition from photoactive α-$FAPbI_3$ to non-photoactive δ-$FAPbI_3$ is pointed as a significant challenge. In addition to phase transition issue, much lower stability of Spiro-OMeTAD is critical for the device performance degradation. As an interlayer in between top metallic electrodes (i.e., Au and/or Ag) and Spiro-OMeTAD/a-$FAPbI_3$, inorganic HTLs prepared by a low-temperature atomic layer deposition (ALD) technique provide bi-functionality to stabilize the PSCs during operation in ambient. Transition metal oxide (TMO) as an inorganic interlayer can be a strong candidate. Most of TMO layers generally require a high processing temperature and the lack of *p*-type characteristics inhibits application to PSCs as hole-transporting interlayers. In this study, we adopt ALD to fabricate TMO layers at low temperatures (~ 50 °C) and intentionally induce oxygen deficient traps to form empty *d*-bands to induce and further enhance hole transporting properties. With their oxygen deficient trap assisted hole transporting properties, we fabricated n-i-p normal structure PSCs of a-$FAPbI_3$ and Spiro-OMeTAD with ALD grown TMOs (amorphous-$TiO_2$, $MoO_x$ and $V_2O_{5-X}$) on top of Spiro-OMeTAD to enhance device stability. During fabrication, we adopt funnel like 2D perovskite passivation layers for defect passivation and enhance perovskite's stability coming from hydrophobic characteristics. [1] As a result, highly efficient PSCs of PCE of over 23% with TMOs are fabricated with pin-hole free hole transporting and protection bi-functional ALD layers. [2,3] The environmental stability of PSCs with ALD-$V_2O_{5-x}$ interlayers is over 90% initial PCE after ~ 600 hrs, while without the interlayer started to be degraded under 80% of initial PCE just after around 200 hrs without any special encapsulation. In conclusion, this study demonstrates the application of TMOs as hole transport/protective bi-functional interlayers and ALD as an optimal deposition method without damaging the underlying perovskite absorber. Furthermore, this study shows the possibility that ALD TMOs can be also applicable to tandem device fabrication with p-i-n type PSCs and stable PSCs' commercialization.

*Keywords: Organic-inorganic metal halides; Perovskite solar cells; Power conversion efficiency; Atomic layer deposition;*

# High-entropy alloy films: a review

**Qing Wang** [1], Xiaona Li, Chuang Dong[1]

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**Abstract**

High-entropy alloys (HEAs), containing multi-principal elements in equimolar or non-equimolar mixing to form simple crystalline structure, have attracted substantial attention for their superior properties and potential applications. The vast compositional space endowed by the multi-principal-element alloying can achieve a synergistic modulation of mechanical and functional properties. As a branch of HEA materials, HEA films exhibit attractive and unique properties, such as high strength and hardness, excellent wear and corrosion resistances, remarkable thermal stability, irradiation resistance, etc., exceeding those of traditional films. In this work, the recent development about HEA films has been generalized. First, the basic concept of HEA films was introduced. Then, preparation methods, composition design, microstructure, various properties, modelling, and simulations were primarily investigated and discussed. And several critical design criteria for achieving prominent properties of the HEA films will be suggested. Finally, the prospects of HEA films will be put forward.

*Keywords: high-entropy alloy films; composition design; microstructure; properties*

# Enhancement of coercivity for Sm(Fe-Co)-based thin films through the infiltration of the elements

**Toshiyuki Shima**[1], Yuichi Mori[2], Soga Nakatsuka[3], Masaaki Doi[4]

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## Abstract

$R$Fe$_{12}$ ($R$: rare-earth elements) compounds with a tetragonal ThMn$_{12}$-type crystal structure are expected to surpass the magnetic properties of Nd-Fe-B sintered magnets, since $R$Fe$_{12}$ compounds possess high saturation magnetization $M_s$ and high anisotropy field $H_A$ by the smallest R/Fe ratio which have high molar fraction among $R_{m-n}$Fe$_{5m+2}$ systems. After the potential superior magnetic properties of Sm(Fe$_{0.8}$Co$_{0.2}$)$_{12}$ thin films were reported, a lot of studies have been performed on these compounds with changing the fabrication conditions to be able to transform these excellent intrinsic magnetic properties to the extrinsic ones, particularly remanent magnetization and coercivity. Recently, we succeeded in realizing a large coercivity of 1.2 T in an anisotropic Sm(Fe$_{0.8}$Co$_{0.2}$)$_{12}$ thin film by adding B, suggesting that the additive element plays an important role in improving the magnetic properties of these compounds.

The samples were prepared by using ultra-high vacuum magnetron sputtering system with base pressure of less than $1.0 \times 10^{-8}$ Pa. The structural analysis was performed by the XRD with Cu-Kα radiation. The magnetization curves were measured by using a superconducting quantum interference device (SQUID) magnetometer, the film composition was determined by EDX.

It was confirmed that addition of B promotes the formation of 1:12 grains surrounded by an amorphous intergranular structure. We have also found that the coercivity can be further increased by elemental infiltration to the grain boundary of the Sm(Fe$_{0.8}$Co$_{0.2}$)$_{12}$ thin films. In this talk, our recent results on the magnetic properties and structure of Sm(Fe-Co) based thin films will be introduced.

*Keywords: SmFe$_{12}$ compound, coercivity, magnet, thin films, grain boundary diffusion*

# Effects of Surface Modification on Primary Water Stress Corrosion Cracking Initiation Behaviour of Nickel-based Alloy

**Seunghyun Kim**[1], Jun-Young Jeon[2], Chang-Young Oh[1]

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## Abstract

Nickel-based Alloy has been extensively used as structural material of pressurized water reactors (PWR) because of its excellence in mechanical properties and corrosion resistance. Among the alloys, however, failures due to primary water stress corrosion cracking (PWSCC) of Alloy 600 have been reported for decades. It is known that PWSCC occurs where weld residual stress, corrosive environments and materials susceptibility co-exist. In this study, as a countermeasure for PWSCC, several surface modification techniques have been applied to introduce compressive stress on the surface of Alloy 600. This study includes ultrasonic nanocrystal surface modification (UNSM), laser peening and e-beam treatment. Using proving ring shape specimen, the surface was modified under tensile stress loading condition with 1.2, 1.5 and 1.8 times of yield strength of Alloy 600. After the modification, residual stress was measured by exploiting X-ray diffraction. PWSCC behaviours of as-received and the surface modified Alloy 600 are being experimentally evaluated under simulated primary water condition (340 °C, 16.5 MPa, 30 cc/kg dissolved $H_2$) and their microstructure and chemistry will examined using TEM and other state-of-the art surface analysis techniques. Up to 1,000 hrs of experiments, PWSCC initiation was observed for Alloy 600 with 1.8 times of yield strength. However, no crack initiation was observed for the modified Alloy 600. The experiment will be continued for 4,000 hrs.

*Keywords: Provide a maximum of 5 keywords which appropriately represent the contents of the presentation.*

# Fuzz evolution of NbMoTaW series multi-principal element alloy films by high-flux He ions irradiation

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## Abstract

Plasma-facing materials under continuous irradiation with high-flux helium (He) ions are often found to develop structures such as He bubbles and fuzz, causing serious damage to the mechanical properties of the materials and pollution to the core plasma. In recent years, refractory multi-principal element alloys (RMPEAs) have attracted much attention due to their inhibitory effect on the evolution of defects. In this study, the growth of He bubble and fuzz in nanocrystalline NbMoTaW and NbMoTaWV RMPEA films is investigated. The specimens were irradiated with 50eV $He^+$ at 1050K to various fluences of $5\times10^{24}$ - $1\times10^{26}$ ions/$m^2$. After irradiation, no growth of fuzz or fuzz-like structures was observed on the surfaces of NbMoTaW and NbMoTaWV RMPEA films, while growth of fuzz and tendrils was observed on the surfaces of tungsten films and NbMoTaW bulks, respectively. The inhibition of fuzz structure of the RMPEA films could be attributed to: (i) High-density columnar crystal grain boundaries provide the absorption and release channels of He. (ii) The sluggish diffusion kinetic effects of RMPEA films suppressed the He diffusion and maintained the He release channels at high temperature. Moreover, NbMoTaWV RMPEA films were discovered to develop smaller He bubbles and less pronounced microcracks than NbMoTaW RMPEA films. It was due to the solid solution incorporation of V which further enhanced the lattice distortion and toughness, as well as the profound suppression of He bubble aggregation.

*Keywords: multi-principal element alloys films, nano-columnar crystal channels, He bubbles.*

# Technical **Oral Session _ Session 4**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 4 (G4)** **10:50 - 12:10, Nov. 21**

**Chair :** Hyung Do Kim (Kyoto University) 303A, 3F

10:50-11:20 **K-G0719** **[Keynote] Thermochemical Hydrogen Production via modified Na-Redox reactions**
Takayuki ICHIKAWA (Hiroshima University, Japan)

11:20-11:40 **I-G0795** **[Invited] Nanostructured hydrides for Hydrogen/Lithium Storage**
Xuebin Yu (Fudan University, China)

11:40-11:55 **O-G0521** **Regeneration and synthesis of Metal Borohydrides - Integration of hydrogen production and storage**
Liuzhang Ouyang (South China University of Technology, China)

11:55-12:10 **O-G0954** **Evaluation of Hydrogen Embrittlement of High Strength Steels in Hydrogen Gas at 0.7 MPa**
Nobuyuki Takahashi (Daido Steel Co., Ltd., Japan)

# Thermochemical Hydrogen Production via modified Na-Redox reactions

**Takayuki Ichikawa**

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**Abstract**

In order to produce hydrogen from renewable energies with a reasonable cost, thermochemical method is attracting a significant attention because mass production effect should be expected. Of course, electrolysis is well known as one of promising methods to produce $H_2$ gas. However, the production cost of $H_2$ by the electrolysis depends on the electricity price (OPEX) and equipment "capacity factor" of electrolyser (CAPEX) even though introduction costs would be low. When we focus on the renewable energy for the hydrogen production by means of electrolysis, a benefit of the mass production is not perfectly expected because of the characteristic properties of its two-dimensionality. Therefore, hydrogen production cost is difficultly decreased by using electrolysis even if the mass production would be attempted.

To expect mass production effect, the reaction cycles for water-splitting based on redox reactions of metallic phase of Na are focused in our group, which is composed of three reactions, that is hydrogen generation by solid-liquid reaction, metal separation by thermolysis, and oxygen generation by hydrolysis. As is well known that sodium oxides, $Na_2O$ and $Na_2O_2$ show highly reactive properties to any kind of metals and ceramics at high temperature conditions around 500 °C, it is quite difficult to control the target reaction, which lead to serious corrosion of the vessel materials. Then, we focus on the reaction mechanism of the thermolysis reaction,

$$2Na_2O \rightarrow Na_2O_2 + 2Na.$$

After the deep investigation such as thermodynamic analyses, we clarified that this reaction was not able to proceed from thermodynamic point of view, indicating that the corrosion reaction played a significant role for this metal separation process. As a modified reaction, metal separation process can be written as follows,

$$2Na_2O + Ni \rightarrow Na_2NiO_2 + 2Na.$$

Some detailed processes of whole water-splitting reaction by using only accessible heat below 500 °C would be given in the presentation.

*Keywords: Hydrogen production; Na redox reactions; non-equilibrium condition, Thermal reduction*

# Nanostructured hydrides for Hydrogen/Lithium Storage

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## Abstract

To implement the hydrogen-based propulsion systems, a viable, high efficient, safe and inexpensive hydrogen storage method is stringently required. The main challenge for hydrogen storage materials to be practical is to release hydrogen at moderate temperature with high contents. Nanotechnology plays an important role in advancing the properties of hydrogen storage materials. In this presentation, we report our latest results on the synthesis, and dehydrogenation properties of a series of hydrogen storage materials that were modified with various nano-templates. These nanoconfined compounds showed favorable dehydrogenation and rehydrogenation performances at ambient temperature, significantly advanced over their corresponding bulk substances. The achieved favorable properties of these materials make them promising candidates for advanced hydrogen storage. Furthermore, some nanostructured hydrides were investigated as anodes and solid electrolytes for lithium-ion batteries.

*Keywords: hydrogen storage; lithium ion batteries; nanostructures; hydrides*

# Regeneration and synthesis of Metal Borohydrides - Integration of hydrogen production and storage

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## Abstract

Hydrogen storage is one of the bottlenecks in the large-scale application of hydrogen energy at present. Metal borohydrides are considered as potential hydrogen carriers via hydrolysis and thermolysis due to their high hydrogen storage density(>10 wt.%). However, their practical application is hampered by their complex synthesis process, high cost, and poor reversibility of hydrolysis. Therefore, the facile, efficient, and inexpensive synthesis and regeneration of metal borohydrides is the precondition to step into practicability.

To close the loop of hydrogen storage, our research group has recently developed a facile, low-cost, and high-efficiency method for synthesizing and regenerating $M(BH_4)_n$(M=Li, Na, and Mg) by mechanochemistry. The hydrated sodium borate ($NaBO_2{\cdot}xH_2O$ ($x$= 2, 4)) and hydrated borax ($Na_2B_4O_7{\cdot}xH_2O$) can react with lost-cost Mg, $Mg_2Si$, $Mg_{17}Al_{12}$, or $MgH_2$ as a solid boron source to synthesize $NaBH_4$ with attractive yields. In particular, $Na_2B_4O_7{\cdot}10H_2O$ and $Na_2CO_3$ formed by the hydrolytic product $NaBO_2$ in aqueous solution reacts with $CO_2$ were ball milled with Mg at room temperature, which realized the regeneration of $NaBH_4$ and the methanation of $CO_2$ at the same time. And this method of converting the B-O bond to B-H bond can also be extended to the regeneration of $LiBH_4$ using $LiBO_2{\cdot}2H_2O$ or $Li_2B_4O_7{\cdot}5H_2O$. Very recently, we also synthesized $Mg(BH_4)_2$ using $MgH_2$ and boron oxides($B_2O_3$ and $H_3BO_3$) at a high yield(close to 80%). In general, this method avoids high-temperature dehydration and expensive hydrogen source, greatly reduces energy consumption and price, and lays a theoretical foundation for large-scale commercial application of borohydrides.

*Keywords: Hydrogen storage; Borohydrides; Mechanochemistry; Borates; Regeneration*

# Evaluation of Hydrogen Embrittlement of High Strength Steels in Hydrogen Gas at 0.7 MPa

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## Abstract

Austenitic stainless steels are widely used because it have excellent resistance to hydrogen embrittlement. On the other hand, martensitic steels, martensitic stainless steels, and precipitation hardening stainless steels, which have high strength, are not selected for a hydrogen gas application due to its poor resistance to hydrogen embrittlement. Recently, the variety of components used in the hydrogen gas environment has been increasing, and increasing of variety of materials used in these components require to be expanded. However, there are not enough data of hydrogen embrittlement behavior of high strength steels. In this study, the hydrogen embrittlement behavior of high strength steels was first evaluated in a relatively low-pressure hydrogen gas environment to investigate the hydrogen embrittlement behavior of high strength steels.

In this study, Slow Strain Rate Tensile (SSRT) tests were conducted on martensitic steels, martensitic stainless steels, and precipitation hardened stainless steels in hydrogen gas at 0.7 MPa and in air, respectively, and the results were compared to evaluate their hydrogen embrittlement behavior. As a result, a correlation was observed between the hydrogen embrittlement behavior and tensile strength. The hydrogen embrittlement sensitivity tended to be mitigated when compared to the results in higher pressure hydrogen gas.

*Keywords: Hydrogen Embrittlement, Martensitic Steel, Martensitic Stainless Steel, Precipitation Hardening Stainless Steel, Hydrogen Gas Environment*

# Technical **Oral Session _ Session 4**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 4 (H4)** **11:20 - 12:30, Nov. 21**

**Chair :** Yasushi Endo (Tohoku University) 303B, 3F

11:20-11:40 **I-H0459** **[Invited] Designing and characterising Al-Si Phase-Transformation-Induced Superconducting ring devices**
Manjith Bose (The University of Melbourne, Australia)

11:40-12:00 **I-H0346** **[Invited] Digital twins of magnetic materials: revealing microstructure-properties correlations**
Bolyachikin Anton (National Institute for Materials Science, Japan)

12:00-12:15 **O-H0090** **Micromagnetic analysis of stripe domain structure of the permalloy lamination with applied strain**
Nam Hoon Goo (Pohang University of Science and Technology, Korea)

12:15-12:30 **O-H0585** **Control of the reaction in Mn/Ga diffusion couple by high magnetic field**
Yoshifuru Mitsui (Kagoshima University, Japan)

# Designing and characterising Al-Si phase-transformation-induced superconducting ring devices

**Manjith Bose[1]**, B. C. Johnson[2], M. Stuiber1[1,3], D. L. Creedon[1], A. Berhane[4], L. H. Willems van Beveren[1], S. Rubanov[5], J. H. Cole[2], V. Mourik[4], A. R. Hamilton[4], T. L. Duty[4], and J. C. McCallum[1]

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**Abstract**

The integration of superconductors with silicon devices is expected to greatly enhance the potential for emerging quantum technologies. By combining both superconducting and semiconducting devices there is promise for investigating topological superconductivity and the potential existence of Majorana fermions. Furthermore, unique architectures may be possible to connect spin qubits with superconducting microwave resonators facilitating qubit coupling over long distances. Hybrid devices are therefore a promising avenue for advancing the field of quantum technology.

There are two primary methods for inducing superconductivity in silicon: non-equilibrium techniques and thermal diffusion. Non-equilibrium techniques involve introducing an exceptionally high concentration of holes into the material, typically through implantation and annealing processes [1]. Conversely, thermal diffusion involves depositing a metal onto the silicon and then inducing the formation of either silicide or alloy through a thermal process [2].

Our recent work presents a process for fabricating a silicon nanowire device on a silicon-on-insulator (SOI) platform [3]. The process involves a thermal inter-diffusion anneal of aluminium contact pads deposited onto the silicon nanowire, which leads to the migration of Al throughout the entire device length scale, leading to the formation of an Al device. This Al device conforms to the original Si device geometry, with a small concentration of Si (<2 at. %). We have conducted low-temperature magnetoresistance measurements on these devices, which demonstrate fluxoid quantization.

*Keywords: Superconductivity, aluminium, nanowires, fluxoid quantization*

1. Shim and C. Tahan, Nat. Commun. 5, 4225 (2014).
2. Ridderbos et al., Nano Lett. 20, 122 (2020).
3. Michael Stuiber, PhD thesis, UniMelb (2019).

# Digital twins of magnetic materials: revealing microstructure-properties correlations

**Anton Bolyachkin[1,2]**, Hossein Sepehri-Amin[1,3], Ekaterina Dengina[1,3], Nikita Kulesh[1], Xin Tang[1,2], Yukiko Takahashi[1], Tadakatsu Ohkubo[1], and Kazuhiro Hono[1,3]

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## Abstract

Magnetic materials are among the prime functional materials in establishing a carbon-neutral society. In particular, high-density magnetic recording media are required in data centers, while permanent magnets are essential components in motors of hybrid/electric vehicles and generators of wind turbines. It is important to improve the performance of such magnetic materials up to their practical limits through fine compositional and microstructural optimization. Micromagnetic simulations are usually incorporated to boost this optimization. These simulations are especially useful when a realistic model of the material can be constructed – a digital twin. Our recent achievements in developing such representative micromagnetic models will be presented in this report. First, a TEM image-based finite element model of FePt granular media allowed us to elucidate the effect of nanodefects on magnetic properties and to realize the micromagnetic approximation of hysteresis loops assisted by machine learning [1,2]. Second, the similar TEM-based approach was used to explain the suppressed coercivity in $SmFe_{12}$-based anisotropic thin films and to guide toward its remarkable enhancement [3]. Finally, the most challenging large-scale finite element model was constructed for Nd-Fe-B hot-deformed magnets based on the FIB-SEM tomographic data obtained for a real sample. With this model, we were able to reproduce the experimental coercivity and to explain its microstructural origins. Thus, the combination of advanced microstructure characterization techniques, state-of-the-art data processing algorithms including machine learning, and GPU-accelerated micromagnetic simulations can bring a new horizon in the design of high-performance magnetic materials.

[1] A. Bolyachkin, H. Sepehri-Amin, I. Suzuki, H. Tajiri, Y.K. Takahashi, K. Srinivasan, H. Ho, H. Yuan, T. Seki, A. Ajan, and K. Hono, Acta Mater. 227, 117744 (2022).
[2] E. Dengina, A. Bolyachkin, H. Sepehri-Amin, and K. Hono, Scripta Mater. 218, 114797 (2022).
[3] A. Bolyachkin, H. Sepehri-Amin, M. Kambayashi, Y. Mori, T. Ohkubo, Y.K. Takahashi, T. Shima, and K. Hono, Acta Mater. 227, 117716 (2022).

*Keywords: micromagnetic simulations, magnetic recording, permanent magnets*

# Micromagnetic analysis of stripe domain structure of the permalloy lamination with applied strain

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**Abstract**

The micromagnetic calculation investigates the stripe domain structure of the permalloy lamination. The influence of the applied strain in the elastic range on the lamination has been controversial. The micromagnetic method provides us with the precise domain configuration, mobile behaviour, and the magnetic hysteresis loops within the given assumptions, which are necessary to understand the changes in magnetic behaviour under strain. In order to calculate stable magnetization, a small hypothetical magnetic volume is prepared to represent the magnetic polarization of the lamination. In the representative volume, the strong anisotropy condition forces anti-parallel alignment between two stripe domains. The time integration of the LLG(Landau-Lifshitz-Gilbert) equation predicts domain configuration and hysteresis loop. The applied strain increases the effective magnetic field by adding magnetoelastic energy. The effective field's increase correlates with the magnetostrictive coefficient and elastic strain tensor. In the GOES lamination, the applied tensile stress increases the field, but the compressive stress reduces it. A sufficient increase of the effective field can eliminate the stray field and enhance the formation of the stripe domains. The tensile strain elevates the field required to activate the magnetic reversal, i.e., the coercive field. The magnetic reversal proceeds with the domain wall motion, and once after the coercive field, the wall motion in tensile strain is faster than that of compressive strain. The compressive strain destroys the stripe domain structure and makes the domain wall motion sluggish. Thus, the compressive strain raises the abnormal iron loss by complex eddy current between lazy domain walls. The tensile strain has a positive effect on removing the stray field domains. However, the tensile stress is unnecessary when the lamination has a solid magnetic anisotropy with highly aligned grains to the field direction because the tensile strain increases the coercive field for domain wall motion.

*Keywords: Magnetic Domains, Micromagnetics, lamination, Eddy current, strain effect*

# Control of the reaction in Mn/Ga diffusion couple by high magnetic field

**Yoshifuru Mitsui**[1], Yumi Watanabe[1], Ryota Kobayashi[1], Rie Y. Umetsu[2], Kohki Takahashi[2], and Keiichi Koyama[1]

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## Abstract

Magnetic field influences the reaction of magnetic materials, which have been studied using diffusion couples [1]. In this study, high magnetic field effect on Mn/Ga diffusion was investigated. Mn/Ga diffusion couples were annealed for 573-773 K in magnetic fields up to 15 T. The effects of annealing temperature and magnetic field intensity on the reaction were investigated.

There was the formation of $Mn_3Ga$, γMnGa, λMnGa, $Mn_2Ga_5$ and $MnGa_4$ phase at Mn/Ga interface after the annealing. At 773 K, the thickness of the λMnGa and $Mn_2Ga_5$ phases did not change by application of 5 T [2]. With increasing magnetic field intensity from 5 T to 10 T, thickness of $Mn_2Ga_5$ phase reduced at 773 K. With decreasing temperature to 673 and 573 K, thickness of these phases was also reduced under 5 T. On the other hand, thickness of Mn-rich phases which included ferrimagnetic $Mn_3Ga$ and ferromagnetic γMnGa did not change by magnetic field [3]. From Arrhenius equation, the activation energy of the reaction of $Mn_2Ga_5$ phase enhanced by magnetic field. It is suggested that the change of activation energy is due to the gain of Zeeman energy of Mn-rich phase. Therefore, magnetic properties of reacted phase were played a key role for such a selective retardation of reaction in Mn/Ga system.

[1] X. Ren, *et al*., J. Alloys Compd. 472 (2009) 525.
[2] Y. Watanabe, *et al*., Mater. Trans. 60 (2019) 2195.
[3] Y. Watanabe, *et al*. J. Alloys Compd. 887 (2021) 161310.

*Keywords: high magnetic field, reaction, ferromagnetic material.*

# Technical **Oral Session _ Session 4**

## **Symposium I :** Biomaterials and Soft Materials and their Application

**Biomaterials and Soft Materials and their Application 4 (I4)** **10:50 - 12:30, Nov. 21**

**Chair :** Hyung-Seop Han (Korea Institute of Science and Technology) 400, 4F

10:50-11:20 **K-I0859** **[Keynote] Zn-based biodegradable metals designed for potential usage within bone**
Yufeng Zheng (Peking University, China)

11:20-11:40 **I-I0941** **[Invited] Zn-Based Alloying Design for Biodegradable Vascular Scaffold**
Hongtao Yang (Beihang University, China)

11:40-12:00 **I-I0797** **[Invited] The Application of Biodegradable Zn-Cu-Ca in Temporary Wound Closure Devices**
Jeffrey Venezuela (University of Queensland, Australia)

12:00-12:15 **O-I0714** **The effect of solute on grain refinement of biodegradable binary Zinc alloys**
NEERAJ SRIVASTAVA (Sardar Vallabhbhai National Institute of Technology, Surat, India)

12:15-12:30 **O-I0391** **NIR-induced corrosion regulation strategy for biodegradable Mg alloy**
You Lv (Huazhong University of Science and Technology, China)

# Zn-based biodegradable metals for potential usage within bone

**Yufeng Zheng**[1]

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## Abstract

Magnesium-based biodegradable metals (BMs) as bone implants have better mechanical properties than biodegradable polymers, yet their strength is roughly less than 350 MPa. In this work, binary Zn alloys with alloying elements Mg, Ca, Sr, Li, Mn, Fe, Cu, and Ag respectively, are screened systemically by in vitro and in vivo studies. Li exhibits the most effective strengthening role in Zn, followed by Mg. Alloying leads to accelerated degradation, but adequate mechanical integrity can be expected for Zn alloys when considering bone fracture healing. Adding elements Mg, Ca, Sr and Li into Zn can improve the cytocompatibility, osteogenesis, and osseointegration. Further optimization of the ternary Zn-Li alloy system results in Zn-0.8Li-0.4Mg alloy with the ultimate tensile strength 646.69 ± 12.79MPa and Zn-0.8Li-0.8Mn alloy with elongation 103.27 ± 20%. In summary, biocompatible Zn-based BMs with strength close to pure Ti are promising candidates in orthopedics for load-bearing applications. Among the newly developed biodegradable metal system (ZnLiSr), Zn0.8Li0.1Sr exhibits excellent comprehensive mechanical properties, with an ultimate tensile strength (524.33 ± 18.01 MPa) comparable to pure Ti (the gold standard for orthopaedic implants), and a strength-ductility balance over 10 GPa%. The in vitro degradation tests using simulated body fluid (SBF) shows that Zn0.8Li0.1Sr manifests a uniform degradation morphology and smaller corrosion pits, with a degradation rate of 10.13 ± 1.52 μm·year-1. Real-time PCR and western blotting illustrated that Zn0.8Li0.1Sr successfully stimulated the expression of critical osteogenesis-related genes (ALP, COL-1, OCN and Runx-2) and proteins. Twenty-four weeks' in vivo implantations within ovariectomized (OVX) rats were conducted to evaluate the osteoporotic bone fractures-treating effects of Zn0.8Li0.1Sr, with pure Ti as control group. Micro-CT, histological and immunohistochemical evaluations all revealed that Zn0.8Li0.1Sr possesses a similar biosafety level to, while significantly superior osteogenesis-inducing and osteoporotic bone fractures-treating effects than pure Ti. Furthermore, based on the antibacterial and osteogenic properties of Zn alloys, Ag and Li were selected as alloying elements to prepare biodegradable Zn-Li-Ag ternary alloys. Li and Ag addition improved the mechanical properties of Zn-Li-Ag alloys. The Zn-0.8Li-0.5Ag alloy exhibited the highest ultimate tensile strength (>530 MPa). Zn-Li-Ag alloys showed strong bactericidal effects on methicillin-resistant Staphylococcus aureus (MRSA) in vitro. RNA sequencing revealed two MRSA-killing mechanisms exhibited by the Zn-0.8Li-0.5Ag alloy: cellular metabolism disturbance and induction of reactive oxygen species production. To verify that the therapeutic potential of the Zn-0.8Li- 0.5Ag alloy is greater than that of Ti intramedullary nails, X-ray, micro-computed tomography, microbiological, and histological analyses were conducted in a rat femoral model of MRSA-induced osteomyelitis. Treatment with Zn-0.8Li-0.5Ag alloy implants resulted in remarkable infection control and favorable bone retention. The in vivo safety of this ternary alloy was confirmed by evaluating vital organ functions and pathological morphologies.

*Keywords: biodegradable metals, Zinc, Zn-Li-Sr alloy,Zn-Li-Ag alloy, bone .*

# Zn-Based Alloying Design for Biodegradable Vascular Scaffold

**Hongtao Yang[1], Yufeng Zheng[2*]**

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## Abstract

Ischaemic heart disease, revealed as the world's NO.1 killer, is responsible for 16% of the world's total death according to the WHO global health estimates. Percutaneous coronary intervention (PCI) using drug-eluting stents (DES) is considered the standard of care to reopen the blocked artery and improve the blood supply of patients. To further improve the efficacy and safety of DES, ultrathin-strut stents are proposed which reduce the strut thickness to less than 70 μm. Biodegradable scaffolds have been proposed to lead the iteration of DES as they provide temporary scaffolding and then disappear, liberating the treated vessel from its cage and restoring normal functions. Nevertheless, too-thick strut has become one of the major challenges of biodegradable scaffolds to achieve intergenerational breakthroughs. Zinc (Zn) has been proven to be one of the promising candidates for biodegradable vascular scaffold considering its favourable degradation behaviour. However, the low strength and brittleness of Zn limit its applications. To improve the comprehensive mechanical property of Zn, a series of prototype Zn alloy systems are designed and fabricated. We find that microalloying with Li, an ultrathin-strut (65 μm) Zn scaffold is accomplished with modified biodegradation behaviour and improved biofunction. The scaffold backbone consists of ultrafine-grained Zn matrix (average grain diameter 2.28 μm), and uniformly distributed nanoscale Li-containing phases. Grain refinement and precipitation strengthening enable the Zn-Li scaffold to achieve twice the radial strength with only 40% of the strut thickness of the pure Zn scaffold. Li alters the thermodynamic formation pathways of products during the scaffold biodegradation by creating an alkaline microenvironment. $Li_2CO_3$ may act actively in stabilizing this microenvironment due to its higher solubility and better buffering capability than products of Zn. Consequently. co-release of ionic zinc and lithium enhance the beneficial differential effects on activities of endothelial cells and smooth muscle cells, which results in a good endothelialization process and limited intimal hyperplasia in porcine coronary artery. Findings here may break the predicament of the next-generation biodegradable scaffolds.

*Keywords: Vascular scaffold, biodegradable metals, Zinc, Alloy design.*

# The Application of Biodegradable Zn-Cu-Ca in Temporary Wound Closure Devices

**Jeffrey Venezuela**[1], Nan Yang[2], Nagasivamuni Balasubramani[3], Rachel Allavena[4], Cora Lau[5], Matthew Dargusch[6]

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## Abstract

A biodegradable zinc-nutrient alloy (Zn-1.0Cu-0.5Ca) was used for the fabrication of subcuticular absorbable staples (SAS). Ultrasonic treatment was used to improve the $CaZn_{13}$ particles' morphology in the cast alloy and enhance the formability and post-deformation strength of the alloy. The alloy's biodegradability in a simulated physiological fluid (Hanks' solution) was confirmed using polarisation and immersion tests. The refined microstructure led to enhanced corrosion homogeneity and resulted in improved strength retention during the immersion test. Initial *in vitro* biocompatibility tests (human umbilical vein endothelial and murine fibroblast cells) indicated the alloy's good biocompatibility.

The Zn-based SAS were created from the hot-rolled alloy using laser cutting. The device was subjected to *in vivo* testing using a small animal model (Sprague Dawley rats), and the commercially available poly(l-lactide-co-glycolide) (PLGA) SAS was used as a comparison reference. The Zn-based SAS successfully closed and healed the incision wound, with outcomes similar to the PLGA staple. Zn also exhibited uniform corrosion, with degradation rates and fixation strength declining steadily over the 12-week *in vivo* test. However, Zn's corrosion rate was considerably slower than the PLGA SAS and such a slow degradation rate may lead to unnecessary implant retention. Additionally, the Zn SAS induced more adverse local foreign body responses due to the metal's stiffness. These findings confirmed the potential of biodegradable Zn for the closure of high-tension and slow-healing wounds.

*Keywords: biodegradable Zn, wound closure device, corrosion, biocompatibility, ultrasonic casting.*

# The effect of solute on grain refinement of biodegradable binary Zinc alloys

**Neeraj Srivastava[1]**, Vedant Bhagwat [2], Banoth Siddu [3], Vuttur Sharathkumar [4], and Choppella S R S S S Venkata Subbarao [5]

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## Abstract

Zn-based biomaterials have great potential to overcome the challenges of Fe and Mg alloys for bioimplant applications due to their moderate corrosion rate and better biocompatibility. However, the ductility (~12%) and yield strength (~20 MPa) of the pure Zn are poor due to fewer slip system. The mechanical properties of pure zinc can be enhanced by adding solute elements using the grain refinement technique.

This study investigates the role of solutes on the microstructure, nucleation behaviour and mechanical properties of binary Zinc alloys. The stir casting technique was used to fabricate the binary Zn-X (X= Mg, Al) alloys. The microstructure and mechanical properties of binary zinc alloys were investigated using optical microscopy and hardness testing. The addition of solutes in the pure zinc metal resulted in grain refinement of the alloy and an increment in hardness of 74%, 63.9%, and 73% when 0.1%, 0.5%, and 1% by weight percentage of Mg in Zn were added, respectively. Similarly, the hardness increased by 62%, 69%, and 44% when 0.5%, 1%, and 2% by wt.% of Al in Zn were added. The grain refinement mechanism of binary zinc alloys was explained by using undercooling behaviour of binary zinc alloys.

*Keywords: Zn-based Biomaterials; Grain refinement; Mechanical property; Cooling curves;*

# NIR-induced corrosion regulation strategy for biodegradable Mg alloy

**You Lv[1],** Mingkun Zheng[2], Zehua Dong[1], Xinxin Zhang[1,*]

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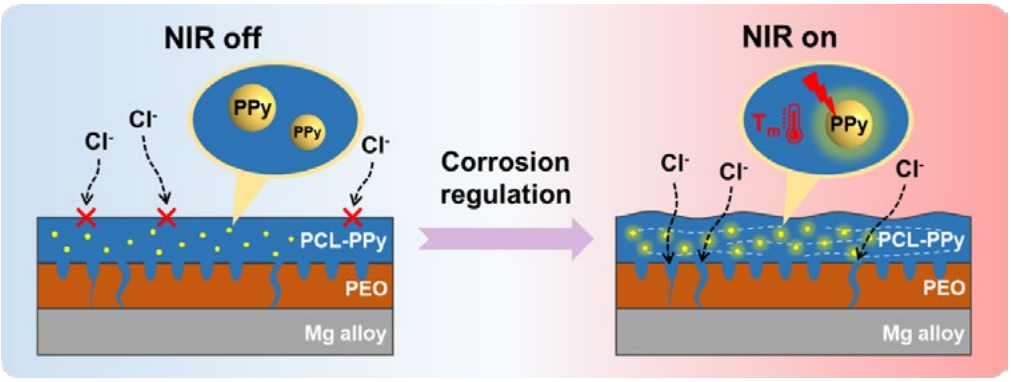
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## Abstract

At present, biodegradable Mg-based implants used in clinical practice have shown high reliability and corrosion resistance, which is hardly degraded in service for more than ten months. However, an overlong degradation period of Mg-based implants increases the risk of infection and the frequency of follow-up for patients. Therefore, controlling the degradation rate of Mg-based implants is an urgent challenge for their clinical application. Herein, we prepare a novel protection system composed of a plasma electrolytic oxidation layer and a polypyrrole-loaded polycaprolactone composite coating on an Mg alloy. During NIR irradiation, the polymer coating integrates binary roles including the NIR response of polypyrrole to achieve the designed temperature, and the transition of polycaprolactone from a rubbery state to a viscous state upon heating. The electrochemical results showed that the system exhibits satisfactory corrosion resistance in simulated body fluid with ~$9.2\times10^{-13}$ A/cm$^2$ of the corrosion current density ($i_{corr}$) and ~$3.3\times10^{9}$ Ω/cm$^2$ of the electrochemical impedance at 0.01 Hz ($|Z|_{0.01\ Hz}$). After NIR irradiation for 1 hour, both $i_{corr}$ and $|Z|_{0.01\ Hz}$ decreased rapidly by 4 orders of magnitude. It was further confirmed by tracking the change of the wettability during the state transition of the coating that the electrolyte rapidly infiltrated into the substrate through the increased molecular chain distance to accelerate its degradation. Hence, this work provides a new strategy for regulating the corrosion rate of Mg-based implants.

*Keywords: near infrared light (NIR); corrosion regulation; state transition; anti-corrosion coating; biodegradable Mg alloy.*




**Scheme 1.** Schematic of NIR-induced corrosion regulation strategy for Mg alloy.

# Technical **Oral Session _ Session 4**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 4 (J4)** **10:50 - 12:30, Nov. 21**

**Chair :** Xiaopeng Li (University of New South Wales) 201B, 2F

10:50-11:20 **K-J1168** **[Keynote] The origin of jerky dislocation motion in high-entropy alloys**
Sang Ho Oh (Korea Institute of Energy Technology, Korea)

11:20-11:40 **I-J0438** **[Invited] Atomic scale in situ observations of the mechanical response of lattice defects**
Eita TOCHIGI (The University of Tokyo, Japan)

11:40-12:00 **I-J0671** **[Invited] Multiple plasticity-enhancing mechanisms of the FeMnCoCr based high entropy alloys**
Jinkyung Kim (Hanyang University ERICA, Korea)

12:00-12:15 **O-J0630** **Substantially enhanced homogeneous plastic flow in hierarchically nanodomained amorphous alloys**
Ge Wu (Xi'an Jiaotong University, China)

12:15-12:30 **O-J0093** **Grain orientation mapping of 1 mm-thick α-Fe by scanning 3DXRD**
Jaemyung Kim (RIKEN, Japan)

# The origin of jerky dislocation motion in high-entropy alloys

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## Abstract

Dislocations in single-phase concentrated random alloys, including high-entropy alloys (HEAs), repeatedly encounter pinning during glide, resulting in jerky dislocation motion. While solute-dislocation interaction is well understood in conventional alloys, the origin of individual pinning points in concentrated random alloys is a matter of debate. In this work, we investigate the origin of dislocation pinning in the CoCrFeMnNi HEA. In-situ transmission electron microscopy studies reveal wavy dislocation lines and a jagged glide motion under external loading, even though no segregation or clustering is found around Shockley partial dislocations. Atomistic simulations reproduce the jerky dislocation motion and link the repeated pinning to local fluctuations in the Peierls friction. We demonstrate that the density of high local Peierls friction is proportional to the critical stress required for dislocation glide and the dislocation mobility.

*Keywords: High entropy alloys (HEAs), Dislocations, Short-range order (SRO), In-situ TEM, X-ray energy dispersive spectroscopy (EDS)*

# Atomic scale in situ observations of the mechanical response of lattice defects

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**Abstract**

Mechanical response of crystalline materials is closely related to the behaviour of lattice defects upon loading. Since the lattice defects such as dislocations, deformation twins, and cracks, are the imperfections at the atomic level, experimental research based on atomic-scale observations can be essential to understand their mechanical behaviour. In situ transmission electron microscopy (TEM) mechanical testing is a powerful technique to directly observe the microstructural changes of materials under loading conditions. However, TEM sample holders for mechanical testing have relatively large machinery parts and thus are not typically compatible with a sample chamber of atomic-resolution TEMs, in which a strong magnetic field is generated within a narrow gap. As micromachining techniques have been advanced in recent years, mechanical devices in micrometer scale, microelectromechanical systems (MEMS), have been put to practical use. MEMS devices can be a promising experimental system for in situ TEM mechanical testing. Indeed, there are several reports on in situ mechanical testing using MEMS devices, although it is still difficult to perform the mechanical testing with atomic-resolution imaging. Here we report mechanical behavior of crystalline materials at the atomic scale by using in situ scanning TEM observations with a custom-made MEMS loading device. Our experimental system successfully produced sequential atomic images of crystalline materials during loading/unloading processes. We will discuss the atomic behaviour and local strain distributions related to the dislocation emission and crack propagation phenomena.

*Keywords: In situ, mechanical test, transmission electron microscopy, crystalline materials, lattice defects*

# Multiple plasticity-enhancing mechanisms of the FeMnCoCr based high entropy alloys

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**Abstract**

The Fe80-xMnxCo10Cr10 high entropy alloys (HEAs) show different phase stability and plasticity-enhancing mechanisms depending upon Mn content. The present work introduces multiple deformation mechanisms observed in the FeMnCoCr-based HEAs. The Fe40Mn40Co10Cr10 alloy exhibits deformation twinning for room temperature deformation and deformation-induced HCP transformation for subzero deformation. Further, at higher strains of subzero deformation, kink banding of HCP and reverse transformation from HCP to FCC were observed, which could account for strain accommodation and stress relaxation, and large ductility. The Fe49.5Mn30Co10Cr10C0.2Ti0.1V0.1Mo0.1 HEA exhibiting less FCC phase stability than the Fe40Mn40Co10Cr10 alloy, show deformation-induced HCP transformation as the main deformation mechanism for room temperature deformation. This material triggers a multi-variant ε phase, reverse transformation from ε to γ, and the multi-step sequential transformation, γ → ε → reverse transformed γ from ε → ε transformed from the reverse transformed γ. The high fraction of deformation-induced HCP plates also contributes to back stress strengthening. The activation of multiple plasticity-enhancing mechanisms in the FeMnCoCr-based HEAs could contribute to the large strain hardening and ductility of the materials.

*Keywords: High entropy alloy; Deformation mechanisms; Deformation-induced HCP transformation; TEM*

# Substantially enhanced homogeneous plastic flow in hierarchically nanodomained amorphous alloys

**Ge Wu**[1]

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## Abstract

In metallic glasses, the plastic deformation is often highly localized in major shear bands at room temperature, inducing strain softening and brittle failure. To alleviate this instability, topologically heterogeneous structures were introduced into metallic glasses to encourage the multiplication of mild shear bands during deformation. Different from the former attentions on topological structure, here we present a compositional design approach to build nanoscale chemical heterogeneity to enhance homogeneous plastic flow upon both compression and tension. To ensure large chemical and consequently mechanical difference between the alternate amorphous nanodomains, i.e. reduce interdiffusion between neighboring amorphous nanodomains during fabrication, positive mixing enthalpy is desired for certain constituent elements of the nanodomains, while negative mixing enthalpy is a precondition to achieve high glass forming ability. These two requirements are reconciled by designing a Ti-Zr-Nb-Si-XX/Mg-Zn-Ca-YY hierarchically nanodomained amorphous alloy, where XX and YY denote other elements. The constituent elements of each nanodomain have large negative mixing enthalpy, while Ti and Mg have positive mixing enthalpy. The received material shows ~2% elastic strain and undergoes highly homogeneous plastic flow of ~40% strain (with strain hardening) in compression, surpassing those of mono- and hetero structured metallic glasses. Furthermore, dynamic atomic intermixing occurs between the amorphous nanodomains during plastic flow, originating from atomic rearrangements via profuse shear transformation events. The intimate mixing prevents possible interface failure, and thus leads to mechanical stabilization of the whole material. Our design of chemically distinct nanodomains and the dynamic atomic intermixing at the interface open up a new avenue for the development of amorphous materials with ultrahigh strength and large plasticity.

*Keywords: Metallic glass, homogeneous plastic flow, hierarchical nanodomain, mixing enthalpy.*

# Grain orientation mapping of 1 mm-thick $\alpha$-Fe by scanning 3DXRD

**Jaemyung Kim**[1], Yujiro Hayashi[2], Makina Yabashi[3]

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## Abstract

Understanding the microstructure of polycrystalline material is of crucial importance in predicting and optimizing the materials' properties. The grain size, grain boundaries, and distribution of defects all play crucial roles in determining the performance and reliability of the material. Many kinds of research have shown that the mechanical strength of polycrystalline metals increases as the grain size decreases to a critical value because grain boundaries act as barriers to dislocation propagation and fatigue crack formation. Additionally, the misorientation angle between adjacent grains can significantly impact the grain boundary energy. Under specific angles and axes, the grains can form a coincident site lattice, resulting in lower grain boundary energy and improved physical and chemical properties. These findings emphasize the importance of understanding the microstructure of polycrystalline materials.

Generally, the grain orientation map was obtained using the electron backscatter diffraction (EBSD) technique. However, it requires a well-polished and conductive surface of the specimen, which leads to the destruction of the specimen during the preparation process. To overcome this limitation, differential aperture x-ray microscopy (DAXM), diffraction contrast tomography (DCT), three-dimensional x-ray diffraction microscopy (3DXRD), high-energy diffraction microscopy (HEDM), and scanning three-dimensional x-ray diffraction microscopy (s3DXRD) have been developed for decades.

Among these methods, s3DXRD microscopy is particularly useful for investigating thick specimens. Small focused x-rays are illuminated to the specimen by rotating and translating the specimen to capture the diffraction spots. By reconstructing the orientation of each voxel, the orientation map of the material can be obtained. The use of conical slits greatly reduces the number of grains in the gauge volume, which increases the spatial resolution and makes scanning 3DXRD ideal for thick polycrystalline materials.

In this presentation, the basic concept of s3DXRD and its application to the 1-mm thick α-Fe steel wire will be addressed. The inverse pole figure map and the completeness map obtained from the ratio between the number of the observed and theoretical diffraction peaks imply that the specimen is composed of a high-dislocation area and low dislocation area.

*Keywords: 3DXRD, scanning 3DXRD, orientation microscopy, IPF, orientation mapping*

# Technical **Oral Session _ Session 4**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 4 (K4)** **10:50 - 12:05, Nov. 21**

**Chair :** Yong ZHANG (University of Science and Technology Beijing) Samda Hall B, 3F

10:50-11:20 **K-K0163** **[Keynote] Welding of high entropy alloys and its use for welding fillers**
Nam Hyun Kang (Pusan National University, Kora)

11:20-11:35 **O-K0105** **High-Temperature Oxidation Behavior of Novel High Entropy Alloys Fabricated via Additive Manufacturing**
Lee Jhuo Lun (National Tsing Hua University, Taiwan)

11:35-11:50 **O-K0985** **Comparative study on various non-equiatomic High Entropy Steel processed by Mechanical Alloying and Spark Plasma Sintering**
Harsh Jain (IIT BHU Varanasi-India, India)

11:50-12:05 **O-K0198** **Solidification of undercooled FeCoNiSn0.95 eutectic high entropy alloy**
Fan Zhang (Northwestern Polytechnical University, China)

# Welding of high entropy alloys and its use for welding fillers

Hyunbin Nam[1], Yoona Lee[2], Sanghyeon Park[3], Sangwon Park[4], Youngsang Na[5], Sun Ig Hong[6], **Namhyun Kang[2]**

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## Abstract

Because high-entropy alloys (HEAs) have excellent mechanical properties owing to the phase stability resulting from their high mixing entropy, these materials have attracted attention as a replacement for structural steel. For an HEA to be used commercially as a structural material, weldability with superior strength is essential, but the tensile strength of HEA welds is significantly deteriorated compared to that of the HEA. Furthermore, the face-centered cubic (FCC)-based HEA has no phase transformation during welding; therefore, tensile fracture occurs based on the grain size of each region (base metal (BM), heat-affected zone (HAZ), and weld metal (WM)) in the welds. For rolled HEAs, because the grain size of the WM is coarser than that of the BM, the mechanical properties of the gas tungsten arc (GTA) weld are worse than those of the BM. Therefore, this study investigates the possibility of welding technology and filler to increase the tensile properties of the transverse-weld joint. Specifically, this study aims to investigate the phase separation with Cu addition and the grain refinement due to the particle stimulated nucleation (PSN) effect and dynamic recrystallization (DRX) on tensile properties to elucidate the mechanism for the improvement in the weld strength.

*Keywords: High entropy alloys, Gas tungsten arc welding, Laser beam welding, Friction stir welding, Fillers*

# High Temperature Oxidation Behavior of Novel High Entropy Alloys Fabricated via Additive Manufacturing

**Jhuo-Lun Lee [1,2,3,5]**, An-Chou Yeh [1,2,3], Hideyuki Murakami [4,5]

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## Abstract

Although additive manufactured high entropy alloys (AMHEAs) have shown potentials to be developed as structural materials for elevated temperature applications, the reported oxidation behaviors of AMHEA were limited, and there is a lack of thoroughly understanding on the oxidation mechanism of AMHEA to-date. In this work, by using thermogravimetric analysis, isothermal oxidation was conducted on two novel AMHEAs at 900°C, 1000°C and 1100°C for 24 hours. For comparative study, traditional Ni-based superalloy IN718 were also prepared by additive manufacturing and tested. For three tested temperature, mass gain curve of AMHEAs showed parabolic trend associated with the formation of protective oxide layer. From 900°C to 1100°C, the weight gains of AMHEAs are all significantly lower than IN718. The oxide layer structure strongly influenced the weight gain behaviour. The results indicate that IN718 can only form $Cr_2O_3$ layer which will gradually decompose beyond 1000°C. By contrast, AMHEAs can form protective $Al_2O_3$ layer. This work can also shed lights on how to further increase oxidation resistance of AMHEAs at elevated temperatures.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: High entropy alloys; Additive manufacturing; High temperature oxidation*

# Comparative study on various non-equiatomic High Entropy Steel processed by Mechanical Alloying and Spark Plasma Sintering

**Harsh Jain[1*]**, Yagnesh Shadangi[2,3], Ashutosh Kumar Dubey[1], N. K. Mukhopadhyay[2]

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**Abstract**

In this study, the structural, microstructural and mechanical properties of various high entrop steel (HES) namely, $Fe_{40}Mn_{19}Ni_{15}Al_{15}Si_{10}C_1$ (HES-1), $Fe_{40}Mn_{14}Ni_{10}Cr_{10}Al_{15}Si_{10}C_1$ (HES-2) an $Fe_{40}Mn_{14}Ni_{10}Ti_{10}Al_{15}Si_{10}C_1$ (HES-3) were investigated systematically. After mechanical alloyin HES-1 exhibited BCC (ferrite), B2-type and γ-brass type phases, whereas in HES-2 & HES-3 th BCC and γ-brass type phases only were observed. The spark plasma sintered samples of HES-1 HES-2 and HES-3 depicted mostly dual phase structures consisting of mostly BCC and FC phases coexisted with the intermetallics, and several carbide and silicide phases. The hardnes value in the SPSed samples of HES-1, HES-2 and HES-3 was evaluated to be 7.8 GPa, 7.4 GP and 10.4 GPa, respectively, whereas the yield compressive strength was 2046 MPa, 1954 MPa an 2305 MPa, respectively. The experimental results on structural, microstructural and mechanic properties of various high entropy steel were correlated with the various thermodynamic parameters, CALPHAD modelling and strengthening mechanisms.

**Keywords:** High Entropy Steel; Mechanical Milling and Spark Plasma Sintering; Structural an Microstructural; Mechanical Properties; Strengthening Mechanism.

# Solidification of undercooled $FeCoNiSn_{0.95}$ eutectic high entropy alloy

**Fan Zhang**, Jianbao Zhang, Ke Hua, Haifeng Wang

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## Abstract

Rapid solidification in undercooled $FeCoNiSn_{0.6}$ eutectic high entropy alloy was observed in-situ by a high-speed high-resolution camera and the microstructures were characterized in detail by scanning electron microscope and electron backscattering diffraction. The study investigated the evolution of the solidification microstructure under rapid solidification conditions with the change of undercooling, and characterized its crystallographic orientation relations. The result shows that the final solidification products were two phases with HCP and BCC structures, respectively. There is a clear variant orientation relation in the phase of BCC structure, resulting from the solid-state phase transition of one of the eutectic products. This process was also confirmed by the DSC results. This work has very important guiding significance for the regulation of the solidification structure, and on this basis, the performance of the material can be improved.

*Keywords: undercooling; eutectic; crystallographic orientation relations*

# Technical **Oral Session _ Session 4**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 4 (L4)** **10:50 - 12:30, Nov. 21**

Chair : To be announced 202B, 2F

10:50-11:10 **I-L0796** **[Invited] Grain Refinement of Cast and Additively Manufactured Aluminum by Heterogeneous Nucleation Site Particles**
Yoshimi Watanabe (Nagoya Institute of Technology, Japan)

11:10-11:25 **O-L0249** **A new evaluation method of martensitic transformation behavior using compositionally graded shape memory alloys**
Hideki Hosoda (Tokyo Institute of Technology, Japan)

11:25-11:40 **O-L0303** **Microstructures and Properties of Diffusion Layer Formed at Laminated Interface of Alumina-Particle Dispersed Magnesium Laminated Compacts Fabricated by MM/SPS Method**
Shigehiro Kawamori (Tamagawa University, Japan)

11:40 -11:55 **O-L0715** **Graphene-coated Ni wires for structural application: Mechanical enhancement and its strengthening mechanism**
Wonjune Choi (Arizona State University, USA)

11:55-12:10 **O-L0805** **Excellent CMAS resistance of a newly developed equiatomic high entropy (Dy1/4Ho1/4Tm1/4Yb1/4)2Si2O7 ceramic pyrosilicate**
Faisal Nazeer (China University of Mining and Technology, Xuzhou, China)

12:10-12:30 **I-L1049** **[Invited] Design and Toughening of High-performance Alloy Coatings and Heat-resistant Aluminum Alloys based on Theoretical Calculations**
Liu Sida (Xi'an Jiaotong University, China)

# Grain Refinement of Cast and Additively Manufactured Aluminum by Addition of Heterogeneous Nucleation Site Particles

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## Abstract

The addition of grain refiners containing potent heterogeneous nucleation site particles promotes formation of a fine equiaxed macrostructure by deliberately suppressing the growth of columnar and twin columnar grains. The commercially available Al-Ti and Al-Ti-B refiners are generally used in most of the aluminum industries for grain refining of aluminum and its alloys. In these refiners, $Al_3Ti$ particles and/or $TiB_2$ particles act as a heterogeneous nucleation site. In my presentation, evaluation methods of lattice matching between heterogeneous nucleation site and crystallized phase are first discussed. It is concluded that M value, which is approximately proportional to the specific misfit strain energy, is potentially applicable to predict the effective heterogeneous nucleation site. Then the concept of grain refiners with high-symmetry $L1_2$ modified $(Al_{1-x}Me_x)_3Ti$ intermetallic compound particles, fabrication method and some results on grain refining performance will be given. The heterogeneous nucleation theory can be applied for additive manufacturening, so called 3D printing. Finally, recent results on grain refinement of additively manufactured commercial purity aluminum by addition of TiC heterogeneous nucleation site particles will be descussed.

*Keywords: Heterogeneous nucleation, Lattice matching, Aluminum, Solidification, Additive Manufacturing (3D printing)*

# A NEW EVALUATİON METHOD OF MARTENSİTİC TRANSFORMATİON BEHAVIOR USING COMPOSITIONALLY GRADED SHAPE MEMORY ALLOYS

**Hideki Hosoda[1],** Taywin Buasri[2], Akira Umise[3], Masaki Tahara[4], Masato Sone[5]

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**Abstract**

Martensitic transformation temperature ($M_s$) as well as its composition dependence are important data for the characterization and design of shape memory alloys. Usually, compositional dependence of $M_s$ has to be evaluated by differential scanning calorimetry (DSC) using various bulk materials with different chemical compositions (hereafter, called "DSC method"). The combinatorial method combined with high-throughput experiment is known as an effective way and that can be done by using compositional (functional) graded materials such as sputtered films (called "combinatorial method"). Recently, we have found that $M_s$ evaluated by the DSC method and the combinatorial method are slightly different each other, and suggested that the difference is caused by the elastic constraint from the neighbour area. Then, a new combinatorial evaluation method to evaluate $M_s$ more correctly is proposed using a combination of compositionally graded materials and a micro-machine technique, and some results for AuTi-CoTi diffusion couple materials are presented.

*Keywords: Martensitic transformation temperature, compositionally graded materials, shape memory alloys, diffusion couple, AuTi*

*a new evaluation method of*
*martensitic transformation behaviour*
*using compositionally graded shape memory alloys*

# Microstructures and Properties of Diffusion Layer Formed at Laminated Interface of Alumina-Particle Dispersed Magnesium Laminated Compacts Fabricated by MM/SPS Method

**Shigehiro Kawamori**[1], Yoshinori Nagai[1], Hiroshi Fujiwara[2]

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## Abstract

20/0/20vol% $Al_2O_3$/Mg laminated spark plasma sintering compacts (20/0/20vol% laminated SPS compacts), which were fabricated by mechanical milling / SPS method, have proved to possess lightweight like that of general practical Mg alloys and higher surface hardness than them. Moreover, the "diffusion layer" formed at their 0/20vol% layer interface has been found to exhibit high adhesion to the 20 and 0 vol% layers. The microstructures and the characteristics of "diffusion layer" were investigated using EPMA, XRD and so on. From the results of XRD, the constitutive phases were identified as αMg and MgO. From the results of microstructure observation and elemental analysis using EPMA at the cross section, the microstructures were presumed to be Al solid-solved αMg, MgO and needle-like $Mg_{17}Al_{12}$ generated along the grain boundary of αMg in the ring-shaped MgO. Furthermore, from the results of microstructural observation and qualitative analysis using TEM of the diffusion layer surface, the needle-like finely dispersed phase estimated to be $Mg_{17}Al_{12}$ is thought to be generated not only near the αMg grain boundary but also at the αMg grain/MgO fine particle interface. The cross-sectional hardness was 145 to 155 HV and was higher than that of the AZ91D Mg alloys. The width grew almost linearly rather than parabolic with the passage of sintering time. It is considered that the solid-state reaction of Mg and $Al_2O_3$ was promoted with the passage of the sintering time, and the amount of Al dissolved from $Al_2O_3$ increased, so that the diffusion amount of Al increased.

*Keywords: 0vol% $Al_2O_3$/Mg laminated spark plasma sintering compacts, microstructures, diffusion layer, hardness of diffusion layer, growth behavior of diffusion layer width*

# Graphene-coated Ni wires for structural application: Mechanical enhancement and its strengthening mechanism

**W. Choi[1],** M. J. Kulak[1], U. Das[1], C. Kim[1], and W. Kang[1,*]

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## Abstract

In this study, the mechanical properties and enhancement mechanism(s) of graphene-coated Ni wires with micro-scale in size were studied. A chemical vapor deposition (CVD) was used to coat the continuous graphene layers on the Ni wire, and the graphene was analyzed quantitatively and qualitatively via Raman and TEM techniques. The tensile tester was designed to measure the micro-scale wire (< 100 μm), including a universal tester for force measurement, a microscope and digital camera for displace measurement, and a sample holder for handling via additive manufacturing. A post-mortem was conducted to measure the displacement using the hundreds or thousands of captured images via the digital image correlation (DIC) method and to synchronize the stress/strain data.

Improved mechanical properties were obtained in the graphene-coated Ni wires; for example, 40% enhanced ultimate tensile strength and 70% improvement in yield strength compared to wires without a graphene layer, which have the same thermal history. We also observed the higher strength efficiency among the graphene/metal composite materials due to considerable mechanical property enhancements and a relatively low amount of graphene layer. Several mechanical strengthening mechanisms will be discussed to explain extraordinary improvements in graphene-coated wires based on numerical calculations and simulations.

*Keywords: Graphene/metal composite, Mechanical property, Strengthening mechanisms, Custom-built tensile tester, Chemical vapor deposition (CVD)*

# Excellent CMAS resistance of a newly developed equiatomic high entropy $(Dy_{1/4}Ho_{1/4}Tm_{1/4}Yb_{1/4})_2Si_2O_7$ ceramic pyrosilicate

**Faisal Nazeer[1,2], Sehreish Abrar[3,4]**

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## Abstract

In this work, novel equiatomic high entropy $(Dy_{1/4}Ho_{1/4}Tm_{1/4}Yb_{1/4})_2Si_2O_7$ or $(4RE_{1/4})_2Si_2O_7$ ceramic pyrosilicate was fabricated through a single solid solution method to use as environmental barrier coating. The SEM analysis of high entropy powders shows the homogenous mixing and XRD proves the formation of single β-phase after milling and sintering. The coefficient of thermal expansion was reported as ($2.3\text{-}4.8\times10^{-6}$ $K^{-1}$) from 400 $K^{-1}$ to 1723 $K^{-1}$. The ultra-low thermal diffusivity (0.4 $mm^2.s^{-1}$) and thermal conductivity (0.8 W/m.˚C) were reported at 1500 ˚C for this novel HE ceramic disilicate. The as fabricated $(4RE_{1/4})_2Si_2O_7$ pyrosilicate shows an excellent CMAS resistant for even up to 48 h and negligible amount of Ca is able to penetrate in the substrate. Rare earth disilicate species with intermediate radii such as $Tm^{3+}$ helps in maintaining phase stability along with passive element $Yb^{3+}$ of smaller radii which also protect the interface from severe CMAS attack. However, the rare earth species with larger radii such as $Dy^{3+}$ and $Ho^{3+}$ actively take part in apatite formation leading to reduced corrosion activity of CMAS melt by changing its composition. This result confirms the application of $(4RE_{1/4})_2Si_2O_7$ as a potential candidate to be used as protecting coating material in harsh combustion environments.

***Keywords:*** *High entropy ceramics; Equiatomic; Rare earth disilicate; Single phase; CMAS; EBCs*

# Design and Toughening of High-performance Alloy Coatings and Heat-resistant Aluminum Alloys based on Theoretical Calculations

**Sida Liu**[1]

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**Abstract**: During the process of alloy material fabrication using magnetron sputtering, the system deviates from equilibrium and easily obtains metastable phases. By combining computational methods such as CALPHAD with experimental techniques, a phase diagram of metastable phases can be constructed for the system, allowing for the investigation of the influence of chemical composition and fabrication processes on material structure, and subsequently evaluating the performance of materials under different structures. For instance, a ternary aluminum-based metastable phase diagram constructed based on CALPHAD and key experiments is used to describe the phase formation behavior of commonly used hard coating material Al-Ti-N in industrial production. Similarly, the construction of a thermodynamic database for the Al-Mn-X system facilitates the understanding of the influence of chemical composition on phase formation in the alloy, thereby providing theoretical guidance for the development of high-strength and tough Al-Mn-based nano-dual phase alloys. This project envisions expanding existing research methods by integrating theoretical calculations, experimental fabrication, electrochemical testing, and advanced characterization techniques to efficiently establish the correlation between composition, structure, and mechanical properties in the Al-Mn system, ultimately leading to the fabrication of high-strength and tough Al-Mn-X alloys.

*Keywords: magnetron sputtering; nano-dual phase; metastable state; thermodynamic calculation*

# Technical **Oral Session _ Session 4**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 4 (M4)** **10:50 - 12:25, Nov. 21**

**Chair :** Seung-Kyun Kang, Seoul National University, Tomotsugu Shimokawa (Kanazawa University) **402, 4F**

10:50-11:20 **K-M1103** **[Keynote] An Integrated Experimental and Molecular Modelling Approach to Investigate Tribological Mechanics in Hot Metal Forming**
Kiet Tieu (University of Wollongong, Australia)

11:20-11:40 **I-M0848** **[Invited] Vacancy-enhanced Twinnability of Cu-In Alloys**
Eun Ae Choi (Korea Institute of Materials Science, Korea)

11:40-11:55 **O-M0218** **Anisotropy in Interfacial Sliding Phenomenon in Cu/Nb ARB (Accumulated Rolling Bonding) Nanolaminates as Revealed by In Situ Synchrotron Microdiffraction – Enabling Atomic Reconfigurations in Interfaces for Stretchable Metallic Conductors**
Arief BUDIMAN (Oregon Institute of Technology, USA)

11:55-12:10 **O-M0319** **Multiscale modelling of the fatigue behavior of accumulative roll bonded Cu/Nb laminates**
Fabien Briffod (The University of Tokyo, Japan)

12:10-12:25 **O-M1007** **Aluminum-Magnesium alloys synthesized by high-pressure torsion for application as anodes in Al-air batteries**
Jorge M. Cubero-Sesin (Costa Rica Institute of Technology, Costa Rica)

# An Integrated Experimental and Molecular Modelling Approach to Investigate Tribological Mechanics in Hot Metal Forming

**Kiet Tieu**[1]

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## Abstract

In the hot rolling process, the surface of a work roll is heated up to 650oC while in contact with the hot steel strips at temperature up to 1100oC. The sliding interface between the work-roll and strip surface are subjected to high pressure/shear loading, speed and temperature. Friction at the strip/roll interfaces during deformation can affect directly the rolling pressure and friction. Roll wear (e.g. oxidation, wear, abrasion, fatigue, etc.) will dictate its working profile and surface finish, the work-roll service life, strip shape and profile.

To reduce rolling friction and roll wear under high pressure/shear, nano-additives and glass lubricants such as alkali phosphates etc, have been introduced to the roll contact to interact with the oxides at high temperature to produce a complex tribofilm at the sliding interface through a mechano-tribo-chemistry process.

This presentation will discuss an integrated approach that involves simulated experiments supported by multi-scale molecular modelling to investigate many tribological aspects in the hot rolling of steel. From the mechano-tribochemistry perspective, it covers the lubrication mechanics of environmentally friendly lubricants that are effective at high temperature, and their beneficial effects on the product quality, oxidative and abrasive wear of the work roll and the strip.

**Keywords:** Tribology, hot rolling, friction, wear, tribo-chemistry

# Vacancy-enhanced Twinnability of Cu-In Alloys

**Eun-Ae Choi**[1], Seung Zeon Han[2], Jee Hyuk Ahn[3], Satoshi Semboshi[4], Sung Hwan Lim[5]

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## Abstract

Twinning-induced plasticity (TWIP) is a method used to strengthen metals by utilizing twin boundaries (TBs) as barriers to dislocation movement. However, pure copper faces challenges in generating deformation twins due to its relatively high stacking fault energy (SFE) of about 50 mJ/m2.

To enhance the strength of Cu alloys through TWIP, additive elements like Al and Zn have been considered to lower the SFE of Cu. However, achieving a sufficient density of TBs under normal conditions is challenging. Severe plastic deformation (SPD) techniques such as equal-channel angular pressing (ECAP) and high-pressure torsion (HPT) have been employed to activate twinning even in Cu-Al and Cu-Zn alloys.

Recent research has demonstrated the presence of high-density deformation twins in Cu-In alloys through normal deformation process, showing excellent yield and tensile strength (~1.3 GPa). However, the effect of indium on the SFE and microstructural changes in copper remains unknown. Understanding the impact of indium on copper's twinnability is crucial for designing copper alloys with TWIP effects.

In this study, we utilized density functional theory (DFT) calculations to investigate the influence of indium on the generation of deformation twins in Cu-In alloys. We compared the twinnability of Cu-In alloys with that of Cu-Al, Cu-Zn alloys, and pure Cu.

Our results indicate that Cu-In alloys exhibit lower twinnability compared to Cu-Al alloys. However, the presence of copper vacancies enhances twinnability, resulting in easier twin generation at low strain rates in Cu-In alloys. This study offers valuable insights for the design of high-strength copper alloys.

*Keywords: Cu-In alloy, Deformation twin, Twinnability, Density Functional Theory, Vacancy*

# Anisotropy in Interfacial Sliding Phenomenon in Cu/Nb ARB (Accumulated Rolling Bonding) Nanolaminates as Revealed by *In Situ* Synchrotron Microdiffraction – Enabling Atomic Reconfigurations in Interfaces for Stretchable Metallic Conductors

**A.S. Budiman[1,2,3]**, R. Sahay[4], N. Raghavan[4], O. Thomas[5], M. Enoki[6]

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## Abstract

Crystallographic anisotropy in elastic properties of nanoscale and other emerging crystalline materials has been widely observed. Their plastic properties – in the form of the interfacial sliding phenomenon in a Cu/Nb nanolaminate fabricated through accumulative roll bonding (Cu(16)/Nb(16) ARB nanolaminate) – were recently reported having similar crystallographic anisotropy dependence using pile-up height measurement with a nanoindentation (Sahay et al., Nanomaterials 2022 [1]). In this study, such crystallographic anisotropy dependence of the interfacial sliding phenomenon in Cu/Nb nanolaminates has been further confirmed using a set of Cu/Nb nanolaminate samples fabricated by Harbin Institute of Technology using similar ARB methodology. Cu/Nb nanolaminate samples in this study are also reported to exhibit strong crystallographic anisotropy associated with the existence of distinct interfaces along the rolling direction (RD) and the transverse direction (TD). To test interface sliding on a macroscale we have developed a shear test based upon a specific sample geometry and on *in situ* tensile loading on an X-ray synchrotron beamline. As received nanolaminate samples exhibit a very anisotropic crystallographic texture as expected from the fabrication process. *In situ* X-ray diffraction in the sheared zone during mechanical loading yields strains in Cu and Nb. Early brittle failure prevents investigating further the sliding at interfaces.

*Keywords: Cu/Nb Nanolaminates, Accumulative Rolling Bonding, Crystalographic Anisotropy, Nanoindentation, Synchrotron X-Ray Microdiffraction*

# Multiscale modelling of the fatigue behavior of accumulative roll bonded Cu/Nb laminates

**Fabien Briffod**[1], Koki Yasuda[1], Takayuki Shiraiwa[1], Manabu Enoki[1]

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## Abstract

Multilayer metallic materials consisting of alternating layers of dissimilar metals with thicknesses that vary from millimeters to nanometers have become increasingly popular as a new design approach for structural materials. These materials offer improved mechanical properties compared to single-phase materials. Recent progress in severe plastic deformation processes, particularly accumulative roll bonding (ARB), has allowed for the creation of bulk nanolaminates, such as copper/niobium (Cu/Nb) nanolaminates. This has opened the door for their use as structural materials. The effect of the ARB process on Cu/Nb composites, including layer thickness distribution, texture development, orientation relationship at interfaces, and mechanical behavior, has been extensively investigated using experimental, theoretical, and numerical methods. For these materials to be suitable as structural materials, it is important to understand not only their deformation behavior but also their failure mechanisms under both monotonic and cyclic loading.

The current study utilizes crystal plasticity finite element (CPFE) simulations to examine the impact of diverse microstructural characteristics on the fatigue properties of Cu/Nb laminates. To achieve this, a phenomenological rate-dependent crystal plasticity model was applied and validated against uniaxial tensile test outcomes. Subsequently, synthetic microstructures were created and subjected to fatigue conditions to analyze the influence of layer thickness and texture.

*Keywords: Cu/Nb, Accumulative roll bonding, Crystal plasticity, Fatigue.*

# Aluminum-Magnesium alloys synthesized by high-pressure torsion for application as anodes in Al-air batteries

Joaquín E. González-Hernández[1], Luis Diego Gutiérrez[2], Diego González-Flores[2], **Jorge M. Cubero-Sesin[1]**

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## Abstract

One of the main challenges for application of aluminum alloys as anodes of Al-air batteries is the self-corrosion in alkaline electrolytes. Al-Mg alloys have shown potential in their electrochemical performance for this aspect, so it is interesting to understand the effects of ultrafine-grained (UFG) structures with high degree of supersaturated solid solution produced by high-pressure torsion (HPT). In this study, Al-3% Mg and 5%Mg have been synthesized from elemental powders under 6 GPa of pressure at room temperature for N=5 and N=30 revolutions. The UFG microstructure improves the resistance towards corrosion in all alloys, moreover with the concentration of 5%Mg, as observed by mass loss and potentiodynamic polarization plots. The Al-5%Mg with UFG structure was included in an in-house designed aluminum-air cell with alkaline gel electrolyte.

*Keywords: high-pressure torsion, aluminum-magnesium alloys, Al-air battery, ultrafine-grained structures.*

# Technical **Oral Session _ Session 4**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 4 (N4)** **10:50 - 12:30, Nov. 21**

**Chair :** Lei Zhang (University of Science and Technology Beijing), Ki Sub Cho (Kookmin University) **203, 2F**

10:50-11:20 **K-N0540** **[Keynote] Deep learning-driven crystallography for inorganic materials**
Keesun Sohn (Sejong University, Korea)

11:20-11:40 **I-N1044** **[Invited] Learning Topological Data Representation and its Applications**
Gang Li (Deakin University, Australia)

11:40-12:00 **I-N0252** **[Invited] Artificial Intelligence for EELS/XAFS**
Teruyasu MIZOGUCHI (The University of Tokyo, Japan)

12:00-12:15 **O-N0486** **Using Unsupervised Learning to Cluster Fatigue Life Based on Small Crack Characteristics**
Katelyn Jones (Carnegie Mellon University, USA)

12:15-12:30 **O-N0323** **Prediction of Macroscopic Mechanical Properties of Heterogeneous Structured Metals Based on Neural Network**
Masaki Nishimura (Tohoku University, Japan)

# Deep learning-driven crystallography for inorganic materials

Byung Do Lee[1], Seonghwan Kim[1], Junuk Ahn[1], Jinhyeok Lee[1], Kyurim Kim[1], Jiyoon Shin[1], **Kee-Sun Sohn[1]**

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**Abstracts**

Synthetic crystallographic data, encompassing both 1D powder X-ray diffraction (XRD) data and 3D electron density data, has been curated for all extant inorganic compounds, thereby paving the way for use in deep learning (DL) applications. The procured data was derived from crystal solutions found in repositories such as the Inorganic Crystal Structure Database (ICSD) and the Materials Project (MP).

In the domain of supervised learning, the 1D powder XRD dataset was utilized for symmetry classification and materials property regression. A diverse array of similarity metrics, including but not limited to Pearson, Spearman, Euclidean, Manhattan, cosine similarity, Jensen-Shannon divergence, dynamic time warping (DTW), and earth mover's distance (EMD), were leveraged to construct 1D powder XRD-based similarity matrices for all ICSD entries. These similarity matrices function in dual capacity: they facilitate K-means clustering while also aiding in the discovery of novel materials analogous to a specific target material. Moreover, generative adversarial networks were employed to achieve style transformation and low-dimensional embedding of 1D powder XRD data.

Two discrete types of 3D electron density data were prepared: the CHGCAR-type dataset, which is an ab-initio calculated density dataset obtained from the MP, and the atomic-scattering-factor-based density dataset driven by X-rays, computed from all ICSD entries. Notably, these 3D electron density datasets were processed using a PointNet to attain symmetry classification and property regression. These 3D electron density data can be deployed for analogous DL tasks as those designed for the 1D powder XRD data.

Relative to diffracted data in reciprocal space, such as structure factor data, 3D electron density in real space offers a more intuitive and direct insight into the materials structure when employed in DL methodologies. However, this approach engenders significant computational demands which are mitigated by harnessing the power of cloud computing infrastructures such as Oracle and KISTI. Despite the requisite high-capacity data storage and costly computational resources like ab-initio calculations, this electron density-based DL strategy is on the cusp of becoming accessible to materials scientists and engineers.

*Keywords: Artificial intelligence, Synthetic powder XRD, Structure factor, 3D electron density data, Deep learning*

# Learning Topological Data Representation and its Applications

**Gang Li**[1], Qian Li[2], Haiyang Xia[3]

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**Abstract**

Topological data analysis (TDA) extracts topological features to quantify the shape of data. TDA has found applications in many fields, including computer vision. In TDA, persistence diagrams (PDs) are topological descriptors of data. However, PDs are not vector so they cannot be directly used in machine learning methods.

Recent efforts have transformed PDs into vectors to enable machine learning tasks (classification, regression, dimension reduction, etc). However, existing methods highly depend on pre-defined polynomials to map PDs to vector representations. This presentation introduces two recent advances in PD representation: polynomial representations and Hilbert space embeddings. These representations could extract more discriminative topological features without requiring pre-defined polynomials.

The representations enable applying various machine learning tasks to PDs and extracting insights from different types of topological datasets. Our work seeks to open new research directions and applications of TDA in chemical/biological science, and materials engineering.

*Keywords: topological data, persistent homology, machine learning, structural analysis*

# Artificial Intelligence for EELS/XAFS

**Teruyasu Mizoguchi**[1]

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## Abstract

The present authors have reported the applications of machine learning (ML) for crystal interface analysis and spectroscopy. For the crystalline interface, the ML approaches, including virtual screening, kriging, and transfer learning, have been used to accelerate structure determination of the crystalline interface [1-3]. Furthermore, the ML approaches have been applied to EELS/XAFS analysis. To develop a method that interpret the ELNES/XANES spectra, hierarchical tree and decision tree methods were combined [4]. In addition to the "interpret" the spectrum, we used an artificial neural network to predict the excited states of the ELNES/XANES from their ground states [5]. The machine learning was also applied to directly predict the materials structure and functions from the spectrum [6].

In the presentation, we will mainly talk on the application of the machine learning for the EELS and XAFS, and briefly touch the resent results on the atomic resolution analysis [7-10].

1) S. Kiyohara et al., *Science Adv.*, **2016**, 2, e1600746, 2) S. Kiyohara et al., *Jpn. J. App. Phys.* **2016**, 55, 045502. 3) H. Oda et al., *J. Phys. Soc. Jpn*, **2017**, 86, 123601, 4) S. Kiyohara et al., *Scientific Reports*, **2018**, 8, 13548. 5) S. Kiyohara et al., *npj Comp. Mater.* **2020**, 6, 68. 6) K. Kikumasa et al., *Adv.. Intel. Sys.*, **2022**, 4, 2100103. 7) T. Miyata et al., *Science Advances*, **2017**, 3, e1701546. 8) Y. Katsukura et al., *Scientific Reports*, **2017**, 7, 16434, 9) K. Liao et al., *Nano Lett.,* **2021**, 14, 10416.

*Keywords: Machine Learning, Artificial Intelligence, EELS, XAFS, Materials Characterization*

# Using Unsupervised Learning to Cluster Fatigue Life Based on Small Crack Characteristics

**Katelyn Jones**[1], Paul Shade[2], Reji John[3], Patrick Golden[4], Elizabeth Holm[5], Anthony Rollett[6]

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**Abstract**

Images of fracture surfaces are rich in information and have long been examined to determine fracture characteristics such as initiation site and crack growth mode. Computer vision and machine learning techniques, including convolutional neural networks (CNNs), are new methods that can be applied to microstructural images to make predictions and connections between the microstructure and material responses. For fatigue failure, a goal is to connect the visual appearance of the fatigue fracture surface to fatigue life.

This work seeks to collect scanning electron microscope (SEM) images of Ti-6Al-4V fatigue fracture surfaces and apply CNNs to build a dataset of fatigue fracture surface images and make a connection between them and fatigue life. Round bar specimens used in a previous study on fatigue life at various stress levels have been imaged in regular intervals with an SEM. The images capture the crack initiation site, short crack, and steady crack regions; multiple magnifications were utilized to determine which length scale allows the machine learning algorithms to infer physically meaningful information. The images are compared using unsupervised machine learning methods to determine which part of the fracture surface provides the information that links the fracture surface to the fatigue lifetime naturally. This will be followed by weakly and fully supervised learning to verify those connections. The images taken, the algorithms used, identified fatigue properties, and fracture characteristics will be presented.

*Keywords: machine learning, fatigue, fractography, computer vision, convolutional neural networks*

# Prediction of Macroscopic Mechanical Properties of Heterogeneous Structured Metals Based on Neural Network

**Masaki Nishimura**[1], Yoshiteru Aoyagi[2]

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## Abstract

Nanoindentation testing is not limited by sample shape or size. It is an efficient and practical alternative to conventional destructive tensile testing, which requires high experimental costs. Some attempts have been made to find a direct correlation between the load-displacement curve of an indentation and the stress-strain curve by introducing the concepts of representative strain and stress. However, conventional research has relied on complicated numerical optimization methods whose accuracy depends on the algorithm's robustness and which are computationally expensive. Moreover, indentation simulation requires consideration of geometrical nonlinearities and complex contact conditions, so computational modeling methods work only under limited conditions and materials. An example of a material whose mechanical properties cannot be estimated by conventional works is a material with locally varying mechanical properties measured by indentation tests. This is because there is no one-to-one correspondence between a load-displacement curve and a stress-strain curve, and it is not easy to relate them using currently proposed physical-mathematical models. To determine a stress-strain relationship from various indentation responses, we focus on neural networks (NNs). NNs are useful in searching for material parameters that relate load-displacement and stress-strain curves because NNs can model complex input-output relationships with high accuracy based on a statistical learning algorithm without using mathematical formulas. In this study, we prepare indentation responses and stress-strain curves from tensile tests of various materials as training data for NNs. We investigate whether predicting macroscopic mechanical properties is possible even for materials whose local mechanical properties vary.

*Keywords: Nanoindentation, Neural network, Mechanical properties, Metals, Stress strain curves*

# Technical **Oral Session _ Session 4**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 4 (O4)** 10:50 - 12:15, Nov. 21

**Chair :** Jong-Hyeon Lee (Chungnam National University), Ichiro Daigo(The University of Tokyo) 401, 4F

10:50-11:20 **K-O1164** **[Keynote] Fundamentals of Chemical Metallurgy for Sustainable Recycling**
Il Sohn (Yonsei University, Korea)

11:20-11:40 **I-O1051** **[Invited] Preferential Dissolution Behavior of Super Duplex Stainless Steel in an Acidic Solution**
Jun-Seob Lee (Changwon National University, Korea)

11:40-12:00 **I-O0760** **[Invited] Mechanisms of alloy and inclusions modulation on corrosion resistance of steels**
Chao Liu (University of Science and Technology Beijing, China)

12:00-12:15 **O-O0915** **Quorum-Sensing Driven Inhibitors for Mitigating Microbial Influenced Corrosion upon Carbon Steel**
Asma Lamin (RMIT University, Australia)

# Fundamentals of Chemical Metallurgy for Sustainable Recycling

Juheon Lee[1], **Il Sohn[2,3]**

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**Abstract**

With limited resources and continued population growth, the demand for raw materials has exceeded its supply. To ensure that consumer needs are met, reuse and recycling of materials and sustainable retrieval of process by-products has become a prerequisite. From end-of-life batteries to steelmaking by-product waste recycling, fundamentals of chemical metallurgy have been essential in developing innovative sustainable recycling technologies. In this work, the thermodynamic and kinetics of process innovations in the recycling of EOL-LIBs (LIFE Process®) and steelmaking process wastes will be discussed and critically assessed. Steelmaking by-product wastes including slags, dusts and sludge will also be identified and discussed in terms of applying the fundamentals of chemical metallurgy. In addition, immobilization of certain heavy metals including Cr will also be discussed and potential solutions addressed.

*Keywords: Chemical metallurgy; Recycling; EOL-LIBs; Steelmaking wastes; Immobilization*

# Preferential Dissolution Behavior of Super Duplex Stainless Steel in an Acidic Solution

**Jun-Seob Lee**

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**Abstract**

Super duplex stainless steels (SDSSs) are widely used for their exceptional corrosion resistance. They consist of equal volume fractions of ferrite (α) and austenite (γ) phases, with a pitting resistance equivalent (PRE) of 40 to 45. To understand the corrosion behavior of SDSSs, it is important to investigate the roles of single-phase electrodes during their coupling. However, separating the two phases from SDSSs is challenging due to their small size. In this study, the preferential dissolution of SDSS in a specific acidic solution was determined using single α-phase and γ-phase specimens, as well as SDSS samples. The galvanic connection behavior between the α-phase and γ-phase was also examined to understand the preferential reaction between the two phases.

*Keywords: Provide a maximum of 5 keywords which appropriately represent the contents of the presentation.*

# Mechanisms of alloy and inclusions modulation on corrosion resistance of steels

**Chao Liu**[1](liuchao@ustb.edu.cn)，Tiqnqi Chen[2]，Xiaogang Li[3]

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**Abstract：**

The importance of research and development of high quality corrosion resistant low alloy steels has become more and more prominent under the common demand of high level of greening economic development and carbon emission reduction in China. Alloying regulation has been proven to be an effective means to improve the corrosion resistance of steel. The adoption of different alloying processes during the smelting process can have a significant effect on the inclusions in the material, which in turn affects the micro-zone chemical-electrochemical mechanism of inclusions inducing local corrosion sprouting. In this study, the micro-zone chemical-electrochemical mechanism of inclusions-induced localized corrosion in steel was systematically investigated using micro-zone electrochemical techniques, first-principles calculations and in situ characterization techniques. The results show that, according to the differences in the physical and chemical properties of inclusions, their induced local corrosion mechanism can be divided into chemical dissolution, electrochemical dissolution (corrosion coupling) and chemical-electrochemical dissolution three inclusions induced local corrosion mechanism. According to the differences in inclusions induced local corrosion emergence mechanism, can reasonably guide the steel smelting process in the selection and optimization of alloying types. For example, in 15-5PH stainless steel, Te treatment can effectively change the physical and chemical properties of MnS inclusions in steel, change the pitting corrosion initiation mechanism of the material, and then optimize the pitting corrosion resistance of the material. In addition, inclusions modulating alloying elements can also have a significant effect on the rust layer or passivation film on the steel surface, which in turn affects the corrosion resistance of the material. For example, during Ca treatment, $CaCO_3$ will be formed in the rust layer by Ca elements, forming an enriched layer to enhance the rust layer densities and improve the corrosion resistance of the material. A small amount of Te can promote the formation of $TeO_3$ in the passivation film and improve the denseness and protection of the passivation film, while an excessive amount of Te will lead to the $TeO_3$ to $TeO_2$ transformation, accelerating the corrosion of the material.

*Key Words：Alloying element modulation; inclusions; localized corrosion; corrosion mechanisms.*

# Quorum-Sensing Driven Inhibitors for Mitigating Microbial Influenced Corrosion upon Carbon Steel

**Asma Lamin,** Anna H. Kaksonen[2], Ivan Cole[3], Paul White[4], Xiao Bo Chen[5]

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## Abstract

Microbiologically influenced corrosion (MIC) is a process in which microorganisms initiate, facilitate, or accelerate the electrochemical corrosion reactions of metallic components. Several reports documented that MIC accounts for about 20 to 40 percent of the total cost of corrosion. MIC in oil and gas pipelines can result in significant loss and serious environmental effects. Biofilm formation due to the presence of microorganisms upon the surface of metal components is known to play a vital role in MIC, which can lead to severe consequences in different environmental and industrial settings. Quorum sensing (QS) system plays a major role in controlling the expression of some bacterial enzymes, like catalase, regulates biofilm formation and thus the MIC rate of metal. As such, avoiding the formation of biofilms through inhibiting QS is a sound strategy for mitigating MIC upon metal surface in engineering services. This research aims to elucidate the mechanistic role of QS in biofilm formation and corrosion of carbon steel X65, a prevalent engineering material for construction of pipelines, through using *Pseudomonas aeruginosa* PAO1 wild type and *Pseudomonas aeruginosa* QS mutant strain as model strains. MIC will be characterised by using a range of electrochemical techniques in conjunction with advanced high-resolution surface analysis. The expected findings will provide new understanding of the role of QS in biofilm formation and inspire new design strategies for controlling MIC through controlling QS activities, which will be applicable to a broad range of engineering practices where MIC is a great threat.

*Keywords: Quorum sensing, quorum quenching, antibiofilm, microbial influenced corrosion*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 5

November 21

14:00-15:30

# Technical **Oral Session _ Session 5**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 5 (A5)** **14:00 - 15:15, Nov. 21**

**Chair :** Jinkyung Kim (Hanyang University ERICA) Halla Hall A, 3F

14:00-14:20 **I-A0468** **[Invited] Hydrogen-assisted crack and embrittlement behavior of medium-Mn steels**
Jeongho Han (Hanyang University, Korea)

14:20-14:40 **I-A1041** **[Invited] Microstructural path and mechanisms of hydrogen-assisted fatigue crack growth of tempered martensitic steels with different tensile strengths**
Motomichi Koyama (Tohoku University, Japan)

14:40-15:00 **I-A0382** **[Invited] Atom probe tomography of hydrogen trapping mechanism in carbide-strengthened steels**
Yi-Sheng (Eason) Chen (The University of Sydney, Australia)

15:00-15:15 **O-A1158** **First-principles study on the P-induced embrittlement and de-embrittling effect of B and C in ferritic steels**
Jingliang Wang (University of Science and Technology Beijing, China)

# Hydrogen-assisted crack and embrittlement behavior of medium-Mn steels

**Jeongho Han**[1], Tak Min Park[1], Hyun Wook Lee[1], Hye-Jin Kim[2]

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## Abstract

In recent years, the steel industry has focused on developing new generations of advanced high-strength steels (AHSSs) to provide steel products that have both excellent formability and rigid structure. Currently, the 3rd generation AHSS is under extensive study for commercialization. Among the potential steels, medium-Mn steels with a lean composition (i.e., Mn < 12 wt%, C < 0.3 wt%, etc.) have gained significant attention due to their reasonable material cost and good mechanical response. The corresponding steel can exhibit a two-phase microstructure with a large amount of retained austenite after intercritical annealing, resulting in high strength and ductility.

However, the commercialization of medium-Mn steels has been hindered by a critical issue known as hydrogen embrittlement (HE). A very low concentration of hydrogen, even at the ppm level, can cause premature failure in these steels. To gain insight into the underlying mechanism of HE and the resistance to it in medium-Mn steels, we systematically summarized the HE behavior of medium-Mn steels and suggested a possible solution to increase the HE resistance of the steels.

**Keywords:** Hydrogen embrittlement; medium-Mn steels; advanced high-strength steels; transformation-induced plasticity.

# Microstructural path and mechanisms of hydrogen-assisted fatigue crack growth of tempered martensitic steels with different tensile strengths

**Motomichi Koyama**[1], Tingshu Chen[1,2], Yuhei Ogawa[3], Hisao Matsunaga[4,5], Eiji Akiyama[1]

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## Abstract

Hydrogen-assisted fatigue crack growth (HAFCG) behavior in tempered martensitic steels with different tensile strengths were investigated by compact tension testing under a 90-MPa hydrogen gas atmosphere. Factors determining the HAFCG paths were tensile strength (TS)-dependent. HAFCG occurred preferentially along prior austenite grain boundaries (PAGBs) with a brittle trend in 1025-MPa-TS steel. Specifically, no significant plasticity evolution was observed around the cracked boundaries with misorientations ranging from 15° to 45°, in which the boundaries were identified as PAGB. That is, hydrogen-enhanced decohesion (HEDE) at the PAGB of the relatively high strength steel was the predominant mechanism of HAFCG. In contrast, 811-MPa-TS steel showed HAFCG predominantly along block boundaries with large plasticity evolution, indicating that the mechanism of HAFCG in lower-TS steel required the assistance of plasticity accumulation during cyclic loadings. A possible role of plasticity accumulation is local strain hardening, which could assist in the occurrence of HEDE at the cracked boundaries, particularly near the boundaries with a misorientation of approximately 60° (i.e., mainly block boundary).

**Keywords:** hydrogen embrittlement; grain boundary embrittlement; martensitic steel; fatigue; crystallography

# Atom probe tomography of hydrogen trapping mechanism in carbide-strengthened steels

**Yi-Sheng Chen**[1,2,3], Pang-Yu Liu[1,2], Ranming Niu[1,2], Hung-Wei Yen[3], and Julie Cairney[1,2]

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## Abstract

The presence of hydrogen in steels can lead to catastrophic embrittlement/early-fracture. This is a serious issue for hydrogen transportation and storage. One possible solution is to incorporate hydrogen traps into microstructure of material, where the knowledge of hydrogen trapping mechanism is crucial for the design of materials with better hydrogen trapping capacity.

In this research, we used atom probe tomography (APT) to examine the hydrogen trapping in two steels with high densities of interphase-precipitating rocksalt-structure titanium carbides (TiC) and titanium-molybdenum-mixed carbides (TiMoC), respectively. We charged the samples with deuterium (D, a hydrogen isotope) to avoid ambiguity from background hydrogen, and we utilized a custom cryogenic sample transfer protocol to allow sufficient signal to be retained for APT observations after D charging. As shown in Figure A from a TiC steel specimen, we found TiCs use their interfaces to trap hydrogen. Whereas the result from a TiMoC steel, as shown in Figure B, exhibits the location of hydrogen trapping is the core of the carbides. These results suggest Mo has a significant effect in altering the hydrogen trapping mechanism in carbide-containing steels, and this effect is likely due to the presence of excess carbon vacancy as a result of Mo addition. The finding could lead to a potential carbide design strategy for increasing the hydrogen trapping capacity in carbide-strengthening steels.

**Keywords:** Steels, Hydrogen Embrittlement, Hydrogen Trapping, Atom Probe Tomography

# First-principles study on the P-induced embrittlement and de-embrittling effect of B and C in ferritic steels

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## Abstract

Grain boundary (GB) segregation significantly modify mechanical properties, among which GB cohesion is of great concern. Phosphorus has been long recognized to cause GB embrittlement in steels and it has been found experimentally that B and C can mitigate the P-induced embrittlement. In the present first-principles study, calculations of ∑5(310) GB in Fe with B, C and P were performed to reveal the mechanism of P-caused embrittlement and de-embrittling effect of B and C. Independent and/or joint effect of B, C and P on the GB energetics and cohesion were determined as a function of concentration. It is found that interstitial segregation sites are more favorable than substitutional sites for all the three elements, and only substitutional P aggravates the GB cohesion, which explains the experimental observation that P only embrittles the GB beyond a critical content. The energetic preference of interstitial B and C makes interstitial P at a disadvantage during site competition, whereas the de-embrittling cannot be simply explained by the intrinsic strengthening effect of B and C. The influence of these elements on the GB cohesion is further interpreted as a net result of mechanical contribution and chemical contribution, which proved to play the dominant role in the embrittling/strengthening effect of substitutional P and interstitial segregants, respectively. It turns out that replacing part of P atoms by B and C can mitigate the strong mechanical distortion, and thus alleviate the P-caused embrittlement.

**Keywords:** Grain boundary embrittlement, First-principles calculations, Ferritic steels, Grain boundary segregation

# Technical **Oral Session _ Session 5**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 5 (B5)** **14:00 - 15:20, Nov. 21**

Chair : Hideyuki YASUDA (Kyoto University), Moon Jo Kim (Korea Institute of Industrial Technology) 301, 3F

14:00-14:20 **I-B0583** **[Invited] High-Temperature Deformation of the Several Quaternary La-based Alloys and their Magnetocaloric Properties after Heat Treatment**
Da Seul SHIN (Korea Institute of Materials Science, Korea)

14:20-14:35 **O-B0359** **Flow Stress Modelling of Alloy720Li during Hot Forging Using Internal State Variables Model**
Jo Nakamura (Tohoku University, Japan)

14:35-14:50 **O-B0256** **Heterogeneous Nanostructure and Mechanical Properties of Cu-Zn system Alloy Bars Produced by Groove Rolling**
Hailun Zhou (Kanazawa University, Japan)

14:50-15:05 **O-B0138** **Investigation of Deformation Temperature Effect on Grain Size of Hypereutectoid Steel**
Dayong Guo (Ansteel Group Corporation, China)

15:05-15:20 **O-B0228** **Study on the optimum thickness of fine grain layer on the surface of continuous casting slab based on hot charging pretreatment process**
Yang Liu (Shougang Group Co., Ltd., China)

# High-Temperature Deformation of the Several Quaternary La-based Alloys and their Magnetocaloric Properties after Heat Treatment

**Kwang Seok LEE[1],** Da Seul SHIN[2]

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## Abstract

Recently, La-based alloys have attracted great attention presumably indebted to the $NaZn_{13}$-type (1:13) cubic structure, promising excellent magnetocaloric effects at room temperature. For the case of La-Fe-Si ternary alloys, hydrogenation heat treatment is inevitable to have magnetocaloric characteristics at room temperature. However, after hydrogenation heat treatment, the structural brittleness of the ternary alloys increases, which implies the limitations of making it a part. In the case of the La-Fe-Co-Si quaternary alloy systems, it has a unique Tc (Curie temperature) at around room temperature and exhibits an excellent magnetocaloric effect without hydrogenation heat treatment, indicating La-based quaternary alloys are expected to relatively be free from the problem of intrinsic brittleness when compared to ternary counterparts. Nonetheless, in order to scale-up into a desired 3D shape, hot forming must be necessarily accompanied. In addition, in order to obtain a magnetocaloric 1:13 phase, appropriate heat treatment should also be performed after hot forming.

In this study, the effect of both the addition of Co and the variation in the composition on the change in the 1:13 phase transformation temperature and subsequent magnetocaloric properties of the La-Fe-Co-Si quaternary alloy was first investigated. As-case $LaFe_{11.2-x}Co_{0.7+x}Si_{1.1}$ (x=0 ~ 0.5) exhibits typical dual-phase-like microstructure, α-Fe and La-rich intermetallic compounds. It was confirmed that the existence of the considerable α-Fe phase is important for hot deformation without fracture at high temperature. By using hot simulator equipped in KIMS, hot rolling with a reduction ratio of up to 68% without fracture and macro-cracks is possible under appropriate conditions. In addition, most of α-Fe and La-rich intermetallic compounds could be phase transformed into $La(Fe, Co, Si)_{13}$ (1:13) phase through heat treatment after high-temperature deformation. However, the optimal post-heat treatment conditions in which the 1:13 phase transformation is possible up to the maximum fraction are drastically sensitive depending on the composition.

*Keywords: La-Fe-Co-Si alloys, High-temperature deformation, Heat Treatment, Magnetocaloric effect, $NaZn_{13}$-type phase*

# Flow Stress Modelling of Alloy720Li during Hot Forging Using Internal State Variables Model

**Jo Nakamura**[1], Nobufumi Ueshima[2], Katsunari Oikawa[3]

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## Abstract

Alloy720Li is a kind of precipitation strengthening Ni-based superalloy and is known as a cast and wrought superalloy for turbine discs in aircraft engines. It is necessary to construct a flow stress model considering the effect of microstructure evolution in order to develop a manufacturing process. The purpose of this study is to establish a flow stress model of Alloy720Li during hot forging by considering the effect of work hardening, dynamic recovery and dynamic recrystallization (DRX) by using internal state variables (ISV) model based on the dislocation theory.

The dislocation density evolution was calculated considering the dislocation generation, dynamic recovery due to glide and climb, and DRX. DRX model accounts for nucleation, grain growth, Zener pinning and solute drag. The flow stress during hot compression was calculated by the sum of work hardening and thermally activated stress. The unknown parameters were determined by minimising the differences between the experimental and calculated values of flow stress, DRX grain size and fraction.

Hot compression tests of Alloy720Li solution-treated at 1104℃ for 4 hours followed by air-cooling, showed that deformation behaviour was clearly changed around 1100 ℃ due to dissolution of tertiary γ' precipitates. We focused on the temperature range of 1100-1150 ℃, where the tertiary γ' precipitates completely dissolved and the primary γ' precipitates remained. In that case, the flow stress and DRX fraction were well predicted by ISV model at strain rate of 0.001-1 $s^{-1}$.

*Keywords: Ni-based superalloy, Hot forging, Flow stress, Dynamic recrystallization, Internal state variables model*

# Heterogeneous Nanostructure and Mechanical Properties of Cu-Zn system Alloy Bars Produced by Groove Rolling

**Hailun Zhou[1],** Chihiro Watanabe[2], Hiromi Miura[3]

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## Abstract

The hot-extruded bar of a Cu-Zn system alloy was subjected to groove rolling. Groove rolling was performed using rolls with grooves of different sizes so that the cross-sectional area of the bars after rolling had octagonal shapes. The specimen bar was rotated by 90 degrees along the axis of the rolling direction after each groove rolling, and rolling was continued up to 68% reduction. With increasing rolling reduction, the initial coarse-equiaxed grains looked macroscopically elongated parallel to the rolling direction. And yet, ultrafine mechanical twins high-densely introduced were found to promptly and drastically fragment the initial grains to develop heterogeneous nanostructure. The tensile strength of the as-hot-extruded bar of 464 MPa increased to 704 MPa after a 42% reduction, and further increased to 940 MPa after a 68% reduction. The remarkable increase in strength is attributed to the evolution of the heterogeneous nanostructure developed by grain subdivision, mainly by mechanical twinning; therefore, it can be concluded that the strength of a Cu-Zn system alloy bar was significantly increased by the evolution of the heterogeneous nanostructure, even with a small reduction of 68%, that is, an equivalent strain of 1.13.

*Keywords: Cu-Zn system alloy, groove rolling, mechanical property, mechanical twinning*

# Investigation of Deformation Temperature Effect on Grain Size of Hypereutectoid Steel

**Dayong Guo**[1], Liguo Ma[2], Hang Gao[3], Bo Zhang[4]

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## Abstract

Hypereutectoid steel wire rods are used extensively to produce wire ropes, steel cords. Microstructures of the wire rods strongly influence the performance of these products. Grain size is one of the important microstructures of wire rods. Homogeneous distribution of the grain size of the hypereutectoid steel is required to ensure the low breakage during wire rod drawing and long fatigue life of the wire ropes and steel cords. However, during the industrial practice, abnormally large grain is sometimes found in the hypereutectoid steel wire rods, which does not meet the quality requirement of the wire rods. High carbon wire rods usually are produced through hot-rolling. The hot-rolling parameters control recovery and recrystallization of high temperature austenite, which controls the final grain size of wire rods. In this paper, the effect of finish rolling temperature on the recovery and recrystallization of high temperature austenite was investigated. It was found that recrystallization didn't occur in the specimen compressed at 800℃. The microstructure of the specimen included some abnormally large grains. When the specimens were deformed at 900℃ and 1000℃, the recrystallization of high temperature austenite was observed, which improved the uniform distribution of the grain size of hypereutectoid steel. The present paper provides important guidance to control the microstructure of hypereutectoid steel wire rods.

*Keywords: grain size, hypereutectoid steel, recovery and recrystallization, hot-rolling*

# Study on the optimum thickness of fine grain layer on the surface of continuous casting slab based on hot charging pretreatment process

**Liu Yang[1]** Wang Wei-hua[1] Zhao Jing[2] Li Xin[1] Xie Cui-hong[2] Zhang Hu-cheng[2]

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## Abstract

Hot charging and hot delivery of continuous casting slabs is an important means of low-carbon, green, energy-saving and consumption reduction for steel enterprises. High temperature hot charging of high-end slabs due to the presence of red delivery cracks on the surface of steel plates has been an important factor affecting the hot charging rate of various steel enterprises.The hot charging pretreatment process is a new process and equipment developed by Shougang Group for the high-temperature hot charging of continuous casting slabs. Through the rapid cooling of the slab surface in the segment of the continuous casting machine, the surface structure of the slab is refined, so as to eliminate the problem of " hot charging crack" on the surface of the steel plate after the high-temperature hot charging of the slab. By means of simulation and process test analysis, the surface stress of casting slab during rolling process is studied. The results show that the surface layer of casting slab needs more than 20mm thick fine crystal layer to avoid " hot charging crack".

**Presenting author**

**Liu Yang,Senior Engineer, Doctor of Iron and Steel Metallurgy, Chief Researcher,Technical Expert of Shougang, long-term engaged in quality control technology research of continuous casting slabs,development of new continuous casting processes, and clean steel smelting.**

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*Key words：Hot charging pretreatment ； Surface fine grain layer；Continuous casting slab*

# Technical **Oral Session _ Session 5**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 5 (C5)** **14:00 - 15:20, Nov. 21**

**Chair :** Ji ZHANG (Central Iron & Steel Research Institute), Katsushi Tanaka (Kobe University) 201A, 2F

14:00-14:30 **K-C0362** **[Keynote] R&D Trends in Mo-Based Ultra-High Temperature Alloys**
Kyosuke Yoshimi (Tohoku University, Japan)

14:30-14:50 **I-C0368** **[Invited] Synergetic Alloying Effects of Mo, V and Zr on the Microstructure and Properties of Multi-elemental Nb-Si Based Ultrahigh Temperature Alloys**
Xiping GUO (Northwestern Polytechnical University, China)

14:50-15:05 **O-C0717** **Elastic moduli and toughness of B1-type (Mo, Ti)Cx in Mo-Ti-C ternary system**
Shuntaro Ida (Tohoku University, Japan)

15:05-15:20 **O-C0887** **Strong enthalpy interaction element modulated microstructure and properties of Cu-Ni-Al alloys**
Yinglin Hu (Dalian University Of Technology, China)

# R&D Trends in Mo-Based Ultra-High Temperature Alloys

**Kyosuke Yoshimi**[1]

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## Abstract

Mo-based alloys are expected to be one of the next-generation ultra-high temperature alloys beyond Ni-based superalloys. In addition to commercial heat-resistant Mo alloys such as TZM and MHC, new classes such as Mo-Si-B, Mo-Si-Ti, Mo-Si-Ti-B, and Mo-Si-B-Ti-C (MoSiBTiC) have been proposed and researched and developed over the past two decades. These new-class alloys are metal-matrix composites in which the Mo solid solution is reinforced with intermetallic compounds and/or ceramics such as $Mo_5SiB_2$, $Ti_5Si_3$, and TiC. The reinforcements are thermodynamically stable against the Mo solid solution and contain Si and/or Ti that can form oxide scales onto the substrate. For these reasons, the new-class alloys have superior high-temperature strength and oxidation resistance to the conventional Mo alloys. On the other hand, their fracture toughness is reduced, especially at low temperatures, due to increased brittle phase(s) volume. Therefore, recent R&D trends in Mo-based ultra-high temperature alloys have focused on simultaneously achieving high-temperature strength, oxidation resistance, and low-temperature fracture toughness. In recent years, the challenge of 3D additive manufacturing has also begun. In the lecture, the R&D trends in Mo-based ultra-high temperature alloys are surveyed, and current achievements are summarized with special attention to the MoSiBTiC alloy.

*Keywords: molybdenum, metal-matrix composites, high temperature strength, fracture toughness, oxidation resistance*

# Synergetic Alloying Effects of Mo, V and Zr on the Microstructure and Properties of Nb-Si Based Ultrahigh Temperature Alloys

**Xiping Guo[1]**, Rui Ma[2], Ping Guan[3]

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## Abstract

Nb-Si based ultrahigh temperature alloys are one potential alternative for Ni based superalloys and can operate at higher temperature (1200~1400 °C) due to their lower densities and excellent high temperature strength. However, their insufficient room temperature fracture toughness and poor high temperature oxidation resistance are the bottlenecks of the practical applications of Nb-Si based ultrahigh temperature alloys. Alloying is an effective way to improve the comprehensive properties of the alloys. It has been reported that alloying with V or Zr in the binary Nb-Si alloy improves the room temperature fracture toughness and high temperature oxidation resistance, while lowers high temperature strength. Considering that Mo element has higher melting point and thus is beneficial for high temperature strength, the present work aims to add Mo, V and Zr simultaneously to improve the comprehensive properties of Nb-Si based ultrahigh temperature alloys.

Fifteen multi-elemental Nb-Si based ultrahigh temperature alloys with nominal compositions of Nb-22Ti-15Si-5Cr-3Al-2Hf-*x*Mo-*y*V-*z*Zr (at.%) were prepared by vacuum non-consumable arc melting. The alloying effects of Mo, V and Zr on the arc-melted and heat-treated microstructures have been investigated. The oxidation performances of fifteen arc-melted multi-elemental Nb-Si based ultrahigh temperature alloys were evaluated at 1250 °C for 1 and 20 h, respectively. The effects of Mo, V and Zr additions on the oxidation resistance of multi-elemental Nb-Si based ultrahigh temperature alloys have been investigated. The microhardness, three points bending and compression at 1250°C measurements were conducted for revealing the effects of Mo, V and Zr additions on the room and high temperature mechanical properties.

*Keywords: Nb-Si based ultrahigh temperature alloy; Phase constituents; Alloying; Molybdenum, vanadium and zirconium; Properties.*

# Elastic moduli and toughness of B1-type (Mo, Ti)$C_x$ in Mo-Ti-C ternary system

**Shuntaro Ida**[1], Kotaro Yonemura[2], Kotaro Hosizaki[3], Xi Nan[4], Nobuaki Sekido[5], Kyosuke Yoshimi[6]

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## Abstract

B1-type MX ceramics are composed of transition metals (M) and C, N, and/or O (X) occupying the M and X sites, respectively, and having M–X nearest neighbor (NN) bonds and M–M and X–X next nearest neighbor (NNN) bonds, exhibit attractive material properties. One drawback of B1-type compounds is their brittleness. Fe–Ti–C alloys containing near-stoichiometric TiC in equilibrium with Fe phase exhibited lower ductility with increasing volume fraction of TiC [1]. However, MX in equilibrium with metal phase can have high degrees of off-stoichiometry, such as in Mo–Ti–C ternary system [2]. Substitution of the elements at M site and the formation of structural vacancies at X site in $MX_x$ can lead to novel properties. Therefore, elastic moduli and toughness of (Mo, Ti)$C_x$ in equilibrium with Mo phase in the Mo–Ti–C ternary system were investigated. The bulk modulus ($K$) of (Mo, Ti)$C_x$ increased with increasing Mo fraction at Ti sites, whereas the Young's modulus ($E$) and shear modulus ($G$) remained almost constant. On the other hand, all the elastic moduli decreased with increasing the fraction of vacancies at C sites. They suggest that the M–X bond strength is the dominant factor in these moduli and the effect of M-M bond on $K$ is greater than that of $G$ and $E$. Alloys on a tie line in the TiC/Mo two-phase region exhibited higher toughness with increasing volume fraction of (Mo, Ti)$C_x$, suggesting that the brittleness of (Mo, Ti)$C_x$ can be improved by off-stoichiometry.

1. S. Ida, K. Watanabe and K. Yoshimi, Tetsu to Hagané 109 (2023) 224–233.
2. S. Ida, N. Sekido, K. Yoshimi, High Temp. Mater. Processes 39 (2020) 164–170.

*Keywords: B1-type (Mo, Ti)$C_X$, Off-stoichiometry, Elastic modulus, Toughness*

# Strong enthalpy interaction element modulated microstructure and properties of Cu-Ni-Al alloys

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## Abstract

Cuboidal γ′ phase coherent precipitation-strengthened Cu-Ni-Al alloys with a softening temperature of 1273K or more than 1273K, high hardness and excellent resistivity thermal stability possess a great potential under high-temperature loads and service environments. However, the γ and γ′ phase is not pure but dissolved with the other elements, which deteriorates the conductivity of alloys. And for the Cu-Ni-Al alloys with higher Cu content, the reduction of the volume fraction of γ′ phase and grain boundary discontinuous precipitation would induce the degradation of heating resistance. In order to solve the above problems, Ti, Nb and V element with strong elemental interaction were introduced into Cu-Ni-Al alloys to investigate the influencing mechanism of trace elements on the microstructure and properties of alloys in detail. The results demonstrate that the addition of Ti, Nb and V element can inhibit the discontinuous precipitation at grain boundary to a certain extent, as well as effectively ameliorating the high temperature properties. The variation in microstructure and properties of alloys at room temperature are related to the additive amounts of elements which should not be excessive. Therefore, multi-component composition design is an effective way to improve the comprehensive properties of Cu-Ni-Al alloy, but the reasonable addition of alloying elements and matching of enthalpy interaction between elements should be controlled.

*Keywords: Cu-Ni-Al alloys; coherent precipitation; discontinuous precipitation; high temperature properties; multi-component composition design*

# Technical **Oral Session _ Session 5**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 5 (D5)** **14:00 - 15:35, Nov. 21**

**Chair :** Shoichi Hirosawa (Yokohama National University)
Yong Hee Jo (Korea Institute Of Materials Science)

Samda Hall A, 3F

14:00-14:30 **K-D1137** **[Keynote] Modelling the influence of hot forging-aging on the multi scale microstructure of Al-Cu alloys using PINNS**
Bernard Rolfe (Deakin University, Australia)

14:30-14:50 **I-D1079** **[Invited] D3Square: A User-Friendly, Data-Driven Machine Learning Platform for Aluminum Alloy Discovery**
Minkyu Park (Virtual Lab, Korea)

14:50-15:05 **O-D0302** **First-principles and experimental study of T1 precipitates in Al-Cu-Li alloys**
MAYA PUTRI AGUSTIANINGRUM (Pohang University of Science and Technology, Korea)

15:05-15:20 **O-D0788** **TEM observation of Al-7%Si-0.3%Mg casting alloy in T5 condition**
Taiki Tsuchiya (University of Toyama, Japan)

15:20-15:35 **O-D0838** **Design of high-strength 7xxx series aluminum alloys via machine learning**
Hyo-Sun Jang (Korea Institute of Materials Science, Korea)

# Modelling the influence of hot forging-aging on the multi scale microstructure of Al-Cu alloys using PINNS

Gaijinliu Gangmei[1,2], **Bernard Rolfe[2],** Santu Rana[3], Kishalay Mitra[4], Saswata Bhattacharya[5]

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## Abstract

Classically the properties of a material are dependent on material structure and processing conditions. To study the effect of process parameters on the microstructure, traditional experiments can be conducted by trial-and-error methods using combinations of processing conditions. But this requires many resources and is an unreasonably large time-consuming task. Therefore, the process designers rely on computational modelling techniques to overcome the challenges associated with experiments. However, given that the microstructural evolution at the intra-grain and inter-grain scale are taking place at different length and time scale, it is difficult to solve them simultaneously in a single physics-based model. Therefore, they are mostly modelled separately at the relevant length and temporal scales. After the models are complete and run can the information between the two scales (inter-grain and intra-grain) then be exchanged at the interface, that is, a resolved-scale based multiscale method. However, physics-based models have high computational costs. One of the emerging strategies that can circumvent the high cost associated with physics-based models involves the use of machine learning to build effective surrogate models. They can accurately predict the microstructure evolution without solving the computationally expensive phase-field evolution equations. Therefore, to overcome the challenges of multi-scale physics-based model, we are developing a robust single surrogate model capable of predicting the structure of a material in response to the processing condition of aging and hot forging while taking both the intra-grain and inter-grain scales into account. The physics at intra-grain and inter- grain scales are learned separately using Physics Informed Neural Network (PINN)-based surrogate models before coupling them together. PINN is chosen as the candidate for the surrogate model as it is built using equations that governs the physics of the phenomena. Moreover, because of its mesh- independent nature, it is ideally suited for scale-bridging problems. Microstructures predicted using our PINN models are verified and validated using the best available public-domain experimental data or with data from large-scale phase-field simulations.

*Keywords: microstructure evolution, material modelling, multi-scale, material informatics.*

# $D_3$Square: A User-Friendly, Data-Driven Machine Learning Platform for Aluminum Alloy Discovery

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## Abstract

Traditional materials design has for centuries been based on a top-down approach characterised by a reliance on experience and trial and error. However, the accelerated pace of technological advancement in today's industrial environment requires a paradigm shift towards the integration of experimental and theoretical techniques. Aluminium, the world's most abundant and widely used lightweight metal, offers superior properties, but the discovery of multi-functional aluminium alloys is a challenging and resource-intensive task.

In this presentation, I would like to introduce "$D_3$Square (Al-Alloy)", a cloud-based platform dedicated to aluminium alloy design. The platform incorporates data-driven machine learning algorithms, with an emphasis on user-centric interfaces and time-efficient machine learning methods. It enables users interested in aluminium alloy design to conveniently predict various material properties in advance, reducing both the time and financial costs associated with traditional methods.

*Keywords: Al-Alloy Design, SaaS, Machine Learning, Inverse Design*

# First-principles and experimental study of T1 precipitates in Al-Cu-Li alloys

**Maya Putri Agustianingrum**[1], Shailendra Kumar Verma[2], Danny Petschke[3], Alireza Zargaran[4], Kyoungdoc Kim[5*]

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## Abstract

We investigate the interfacial thermodynamic stability of T1 phase and strengthening effects in commercial aluminum-lithium (Al-Li) alloys using a first-principles density-functional theory calculation. We find that (i) the presence of Cu atoms at T1/Al interface is due to segregations of solute Cu atoms at the interface, and (ii) the semi-coherent interfacial energy of T1/Al interface shows 0.693-0.770 J/m$^2$ depends on interface terminations in atomistic-scale. (iii) Compared to δ' and θ' precipitates in Al alloys, the T1 phase is the most strengthener by comparing the two-modified Al-Li alloys (Cu/Li ratio variations) versus commercial aluminum alloys of AA2195. This work will shed light on the multi-scale modeling of T1 precipitates, ultimately, designing high-performance of Al-Cu-Li alloys using Integrated Computational Materials Engineering (ICME).

*Keywords: aluminum alloys; precipitation; density functional theory (DFT); first-principles calculation; scanning/transmission electron microscopy (STEM); strengthening.*

# TEM observation of Al-7%Si-0.3%Mg casting alloy in T5 condition

**Taiki Tsuchiya**[1], Seungwon Lee[2], Susumu Ikeno[3] and Kenji Matsuda[4]

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## Abstract

Al-Si alloys have been used as casting materials for automobile parts. Al-Si-Mg alloys enhance its strength due to precipitation of metastable phase. However, precipitation sequence is not clear in T5 condition. The aim of this work is to estimate mechanical properties and to classify precipitates by Micro Vickers hardness measurement and microstructure observation of Al-Si-Mg alloy in T5 condition. Alloy was fabricated by casting using iron mould having Y-shape cavity. Alloy was cooled in the mould and temperature was measured. When temperature drops to 773K, alloy was quenched into ice water. After casting, artificial aging was carried out at 473K. Micro Vickers hardness measurement was performed using Mitutoyo HV-101 (load: 0.98N, duration time:15s). Microstructure observation were performed using Optical Microscopy (OM, OLYMPUS BX51M), Scanning Electron Microscopy (SEM, HITACHI S-3500H) and Transmission Electron Microscopy (TEM, TOPCON EM-002B). As the result of TEM observation in peak aged condition, There were needle-shaped precipitates along <100>Al direction and granular-shaped precipitates. The distribution of needle-shaped precipitates and granular-shaped precipitates were different from place to place. We analysed needle-shaped precipitates and granular-shaped precipitates with HRTEM images and SAED patterns. It was confirmed that needle-shaped precipitates were β'' phase and granular precipitates were Si phase.

*Keywords: Al-Si-Mg alloy, Aging, Precipitation, TEM observation*

# Design of high-strength 7xxx series aluminum alloys via machine learning

**Hyo-Sun Jang**[1], Hyun-Seok Cheon[2], Jisu Kim[3], Su-Hyeon Kim[4], Jiwon Park[5], Chang-Seok Oh[6]

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## Abstract

As the demand for high-strength materials for transportation equipment such as automobiles increases, the need for developing new aluminum (Al) alloys that overcome the limitations of existing commercial Al alloys is growing. In this study, to meet these needs, high-strength Al alloys were explored using machine learning. To this end, we selected papers on 7xxx series Al-Zn-Mg alloys that show high strength among existing Al alloys and collected data such as bibliographic information, alloy composition, process conditions, and mechanical properties. Next, data pre-processing such as filling missing data and removing outliers was performed to perform machine learning with the collected data. Feature selection was also performed to select the main factors to be used in machine learning through correlation analysis. Using this data, we searched for a forward machine learning model that best predicts the strength of Al alloys and derived the composition and process conditions of Al alloys with a tensile strength of 700 MPa or more through reverse design using genetic algorithms. Its consistency was then confirmed through experiments.

*Keywords: Aluminum alloys, Machine learning, Inverse learning, Ultimate tensile strength*

# Technical **Oral Session _ Session 5**

## **Symposium E :** Additive Manufacturing

### Additive Manufacturing 5 (E5) 14:00 - 15:35, Nov. 21

**Chair :** Cecilie Funch (The University of Sydney), Takayoshi NAKANO (Osaka University) Halla Hall B, 3F

14:00-14:30 **K-E0309** **[Keynote] Elastic properties of additively manufactured biomedical Ti alloys**
Masakazu TANE (Osaka Metropolitan University, Japan)

14:30-14:50 **I-E0091** **[Invited] Hetero-microstructure effect on the mechanical and corrosion properties of directed energy deposition-processed Ti-Zr-Nb-Sn alloy**
Jung Gi Kim (Gyeongsang National University, Korea)

14:50-15:05 **O-E0636** **A Comprehensive Study on Process Optimization, Defect Investigation, and Aging Analysis of 18-Ni 300 Maraging Steel Processed via Selective Laser Melting**
Biranchi Narayan Sahoo (Sardar Vallabhbhai National Institute of Technology, Surat, India)

15:05-15:20 **O-E0514** **Effect of post-heat-treatment on microstructures and mechanical properties for D2 tool steels fabricated via direct energy deposition**
Heechan Jung (Korea University, Korea)

15:20-15:35 **O-E0380** **Dynamic strength of additively repaired stainless-steel under high strain-rate loading**
Jesse Callanan (Los Alamos National Laboratory, USA)

# Elastic properties of additively manufactured biomedical Ti alloys

**Masakazu Tane[1],** Shota Higashino[2], Daisuke Miyashita[3], Eisuke Miyoshi[4] , Takuya Ishimoto[5] , Takayoshi Nakano[6]

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## Abstract

Additively manufactured $\beta$-phase Ti alloys with a body-centered cubic (bcc) lattice have attracted considerable attention for use in biomedical applications, such as artificial hip joints and dental implants. This is because $\beta$-phase Ti alloys have a low Young's modulus, which is necessary to prevent bone degradation and absorption resulting from the difference between the Young's moduli of the implants and natural human bone. However, the effects of microstructures formed by additive manufacturing on the elastic properties have not been revealed in detail. In the present work, we studied the elastic properties of $\beta$-phase Ti alloys prepared by selective-laser-melting-type additive manufacturing. To reveal the effects of anisotropic microstructure formed by the additive manufacturing on the elastic properties, the anisotropic elastic properties, which reflect the anisotropic microstructures, were measured using resonance ultrasound spectroscopy. Furthermore, we analysed the correlation between the anisotropic elastic properties and microstructures using the Voigt-Reuss-Hill approximation and micromechanics-based methods. These analyses revealed a potential strategy for designing additively manufactured $\beta$-phase Ti alloys with a low Young's modulus.

*Keywords: Elastic properties, Additive manufacturing, Biomedical materials*

# Hetero-microstructure effect on the mechanical and corrosion properties of directed energy deposition-processed Ti-Zr-Nb-Sn alloy

**Jung Gi Kim[1],** Yukyeong Lee[1], Shuanglei Li[2], Taekyung Lee[3], Jeong Seok Oh[1], Jun-Seob Lee[4], Tae-Hyun Nam[1]

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## Abstract

Ni-free $\beta$-type Ti alloys have been developed to manufacture high-strength, low-elastic-modulus, shape-memorable medical, and non-toxic components. Because the machinability of these alloys is generally poor, processing via additive manufacturing is an important step in the development of order-made medical devices. Although many studies evaluated the mechanical properties of additively manufactured Ni-free $\beta$-type Ti alloys, investigation of their heterogeneous microstructure resulting from the rapid melting-solidification cycling during laser scanning has not been discussed yet. In this study, the role of a heterogeneous microstructure on the performance of a directed energy deposition-processed Ti-Zr-Nb-Sn alloy was investigated. The metastable and nanosized ω phase, which is initiated in the non-equilibrium environment, enhances the yield strength without severe ductility degradation. Additionally, deformation-induced martensitic transformation occurs near the unmelted particle/matrix interface, and this phase transformation not only contributes to transformation-induced plasticity but also provides superelasticity to the present alloy. In particular, unmelted Nb particles, which are homogenously distributed in the matrix, do not critically affect the local corrosion behavior because of their low contact potential difference with the matrix. The results show that the heterogeneous microstructure of the directed energy deposition-processed Ti-Zr-Nb-Sn alloy exhibits outstanding mechanical properties and superelasticity, while its corrosion is marginal that can be sustained in the human body.

*Keywords: Additive Manufacturing, Titanium, Shape Memory Alloy, Mechanical Property, Corrosion*

# A Comprehensive Study on Process Optimization, Defect Investigation, and Aging Analysis of 18-Ni 300 Maraging Steel Processed via Selective Laser Melting

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**Abstract**

Maraging steel (MS-300) finds wide applications in the marine, automobile, aerospace, tooling, and molding industries. Its flexibility in manufacturing has been enhanced through the Selective Laser Melting (SLM) process, which allows for the manufacture of complex shapes, reduces waste material, and offers good mechanical and microstructural properties. The objective of this research is to enhance the newly integrated SLM process by utilizing the response surface methodology's Central Composite Design (CCD) tool to optimize its parameters for MS300. The process parameters considered are laser power, scanning speed, hatch space, and layer thickness, which are optimized to achieve high density and low surface roughness. The study concludes that the optimal process parameters for MS-300 are a laser power of 200W, scanning speed of 600 mm/s, hatch space of 0.1mm, and layer thickness of 40µm, resulting in a density of 99.12% and surface roughness of 5.94µm. The study also investigates defects such as keyhole, balling effect, cracks, and porosity, as well as laser tracks and layers due to parametric variation. To enhance the mechanical properties of SLM-fabricated MS-300, post-heat treatment, including solution treatment and aging, are employed. The generation of precipitates mechanism is established through Johnson–Mehl–Avrami (JMA) equation. Furthermore, detailed microstructure characterization is carried out to gain a better understanding of under-aging and over-aging concepts and determine the factors contributing to the enhancement of mechanical properties after aging.

***Keywords:*** *Selective Laser Melting, MS 300, Aging behavior, Microstructure, Mechanical properties.*

# Effect of post-heat-treatment on microstructures and mechanical properties for D2 tool steels fabricated via direct energy deposition

**Heechan Jung [1]**, Seungjin Nam[1], Hyun Chung[1], Chahee Jung[2], Hyunjoo Choi[2], Seok Su Sohn[1]

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## Abstract

D2 tool steel is widely recognized for its exceptional hardness and excellent wear properties, primarily due to its martensite matrix reinforced with eutectic carbides obtained through conventional heat treatment. Considering the increasing demand for complex-shaped D2 tool steel parts, additive manufacturing has emerged as a promising method for their fabrication. Nevertheless, the as-built state of D2 tool steel fabricated via additive manufacturing does not possess the desired properties, as the matrix remains in the FCC phase rather than transforming into martensite during deposition. Considering the inherent differences in microstructure and phase stability between additive manufacturing materials and traditional cast or wrought materials, it is required to adjust microstructures through controlling heat-treatment conditions. In this study, the post-heat-treatment under various conditions was applied to the D2 steel fabricated using the laser-direct energy deposition (L-DED) method. Detailed investigations on the microstructure and hardness enhancement according to the carbide and martensite fractions will be introduced.

*Keywords: D2 tool steel; Additive manufacturing; Heat treatment; Hardness;*

# Dynamic strength of additively repaired stainless-steel under high strain-rate loading

**Jesse Callanan**[1], David Jones[2], Daniel Martinez[3], Kendall Hollis[4], Saryu Fensin[5]

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## Abstract

Improvements in metal additive manufacturing have led to new possibilities in for repairing high-value components. Making repairs has the potential to reduce overall cost, reduce downtimes, and expand the range of options for application and material types, however there is a lack of quantitative understanding of the mechanical behavior of such repairs under high pressure, high strain rate loading. In this work, artificially damaged stainless-steel samples were repaired with additive manufacturing technology and the mechanical properties were investigated. Several types of damage sites on the order of one cubic millimeter were inflicted on samples to replicate damage commonly incurred during manufacturing or regular use of metal parts. The damage sites were repaired with pulsed laser deposition additive manufacturing, and the repaired samples were tested at dynamic strain-rates. Post-mortem metallography was used to study the links between repair processing methodology, microstructure, and mechanical performance. Results show that optimal process parameters are critical for realizing effective repairs due to the dependence of damage morphology on the resulting microstructure.

*Keywords: additive manufacturing repair, shock loading, dynamic strength, stainless steel*

Topic area: E, Additive Manufacturing

# Technical **Oral Session _ Session 5**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 5 (F5)** **14:30 - 15:30, Nov. 21**

**Chair :** Michihisa FUKUMOTO (Akita University), Toshiyuki SHIMA (Tohoku Gakuin University) 202A, 2F

14:30-14:45 **O-F0341** **Changes in Existing States of Hydrogen in Electrodeposited Palladium Films by Bath Temperature**
Tomoya Hashimoto (University of Hyogo, Japan)

14:45-15:00 **O-F0595** **Microstructure and thermal shock resistance of self-healing thermal barrier coatings modified by laser surface treatment**
Panpan Zhang (Zhejiang University of Technology, China)

15:00-15:15 **O-F0746** **Self-organized nanohole: formation, characterization, and properties**
Hiroaki Tsuchiya (Osaka University, Japan)

15:15-15:30 **O-F0578** **Laser assisted electrochemical surface modification of titanium alloys**
Guolong WU (Zhejiang University of Technology, China)

# Changes in Existing States of Hydrogen in Electrodeposited Palladium Films by Bath Temperature

**Tomoya Hashimoto[1],** Naoki Fukumuro[2], Shinji Yae[3]

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## Abstract

Electrodeposited palladium (Pd) films are widely applied to surface finishing. Co-deposited hydrogen in the Pd films affects their functional and aesthetical properties. In this study, we investigated the structural changes in the Pd films with the desorption of co-deposited hydrogen, and the atomistic states of hydrogen in the Pd films.

The Pd films were electrodeposited from an alkaline bath consisted of palladium (II) chloride, ammonium chloride, and citric acid. The electrodeposition was carried out at 298 K and 278 K with a constant current density of 50 A $m^{-2}$. A stainless steel plate (SUS304) was used as a substrate. The co-deposited hydrogen in the Pd film was analysed by thermal desorption spectroscopy, and the structural analysis were performed by X-ray diffraction and transmission electron microscopy.

In the Pd films electrodeposited at 298 K, hydrogen desorption peaks ascribed to the break-up of vacancy-hydrogen clusters and the desorption of hydrogen molecules from nano-voids were observed in the thermal desorption spectrum of hydrogen. The lattice parameter was smaller than that of standard Pd sample, and the lattice contraction proceeded concurrently with hydrogen desorption at room temperature. On the other hand, in the Pd films electrodeposited at 278 K, a new pronounced peak ascribed to the desorption of interstitial hydrogen appeared at around 350 K, and the lattice expansion was observed. These results indicated that the atomistic states of hydrogen in the Pd films changed depending on the bath temperature.

*Keywords: Hydrogen Co-Deposition, Interstitial Hydrogen, Hydrogen-Induced Superabundant Vacancies, Nano-Voids, Thermal Desorption Spectroscopy*

# Self-organized nanohole: formation, characterization, and properties

**Hiroaki Tsuchiya, Sayaka Miyabe, Shinji Fujimoto**

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## Abstract

Self-organization phenomena have attracted much attention not only from scientific but also from technological points of view. In the field of electrochemistry, nanoporous and nanotubular structures have been extensively studied: porous alumina, titania nanotubes. The nanoporous and nanotubular oxide layers can be grown by self-organizing anodization under suitable electrochemical conditions. Recently, nanoporous and nanotubular oxide layers have been reported not only on Al and Ti but also other valve metals and alloys such as Ti alloys and stainless steels. In the case that the functions of the nanoporous and nanotubular oxide layers are not utilized in practical applications, the formation of nanoporous and nanotubular oxide layers is not necessary. Instead, dimple arrays that are formed under the nanoporous and nanotubular oxide layers can be used for the other applications than those reported for nanoporous and nanotubular oxide layers. Although such structures can be obtained by removing the nanoporous and nanotubular oxide layers, we present in the present work direct formation of dimple arrays, so-called nanohole structure on Cr-containing alloys such as stainless steels, Inconel and Co-Cr alloy. Their characterization and properties are also briefly addressed.

*Keywords: Electrochemistry, Nanohole, Self-organization, stainless steel, Co-Cr alloy*

# Laser assisted electrochemical surface modification of titanium alloys

**Guolong Wu[1,2],** Lin Li[1,2], Zhenzhen Yang[1,2], Ye Wang[1,2], Jianhua Yao[1,2]

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**Abstract**

Laser assisted electrochemical surface modification (LESM) technology is a general term for coupling laser and electrochemical treatment technology to improve the surface properties of metal. Due to combining the advantages of laser and electrochemical processing, LESM has developed rapidly in recent years and gets applications in many fields, such as aerospace, aviation, navigation, and medicine. On the one hand, LESM can break through the limitations of single processing in environmental protection, efficiency, quality, and performance improvement. On the other hand, it can use the thermal, mechanical, and photoelectric effects provided by laser irradiation to change the thermodynamics and dynamics of the electrochemical reaction, and then control the electrochemical reaction process. LESM enables divided into three types based on the processing objective, including material removal (electrochemical machining), additive manufacturing (electrodeposition), and surface strengthening treatment (anodic/ micro-arc oxidation). Simultaneously, according to the composite mode, it can also be divided into process composite and energy field composite. Thus, the typical methods of LESM are reviewed in this paper, and the recent developments in laser-assisted electrodeposition, laser-assisted electrochemical machining, and laser-combined micro-arc oxidation technologies are introduced at the same time. Finally, the future development trends and challenges of LESM prospect in aspects of efficiency, quality, performance, and equipment development.

*Keywords: Laser surface engineering; electrochemical surface modification; micro-arc oxidation*

# Technical **Oral Session _ Session 5**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 5 (G5)** **14:00 - 15:30, Nov. 21**

Chair : Hyung Do Kim(Kyoto University) 303A, 3F

14:00-14:30 **K-G0541** **[Keynote] Hydrides for energy storage and conversion**
Ping Chen (Dalian Institute of Chemical Physics, China)

14:30-14:45 **O-G0522** **The synergistic effect of Ni and Pd for Boosting the hydrogen storage performance of MgH2**
Shaoyang Shen (South China University of Technology, China)

14:45-15:00 **O-G0543** **Surface structures and hydrogenation properties of Ti-Pd alloys immersed in hydrogen peroxide**
Ryota Kondo (Kansai University, Japan)

15:00-15:15 **O-G0718** **Disproportionation of Ti4Ni2Ox (x=0-1) in H2 atmosphere**
Yuki Kashiyama (Kasai University, Japan)

15:15-15:30 **O-G0726** **LaNi5 Metal Hydride as a Catalyst for Liquid Organic Hydrogen Carrier**
Sung Ju Han (Korea Institute of Science and Technology, Korea)

# Hydrides for energy storage and conversion

Teng He, Hujun Cao, Jianping Guo, **Ping Chen**

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## Abstract

Metal hydrides (MH) exhibit unique chemical and physical properties that are essential to energy storage and chemical transformation. In this talk, I will show the development of MH for hydrogen storage and hydride ion conduction, and the roles of MH in mediating ammonia synthesis.

Chemical hydrogen storage is a grand challenge in the implementation of hydrogen energy system. Our work shows that MH reacts with ammonia, ammonia borane, phenol and carbazole etc., forming a variety of composite or complex hydrogenous compounds that possess interesting hydrogen storage properties.

Ammonia is a hydrogen carrier. Alkali or alkaline earth metal hydrides serve as electron and H donors. They actively involved in the activation and conversion of dinitrogen and change the scenario of catalytic ammonia synthesis.

Materials that conduct pure hydride ion will be an enabler of advanced clean energy storage. By creating grain boundaries and defects in the lattice of lanthanum hydrides, its electronic conductivity can be suppressed by more than 5 orders of magnitude. This transforms $LaH_x$ to a superionic conductor at -40 °C with a record high hydride ion conductivity of $1.0 \times 10^{-2}$ S $cm^{-1}$ and a low diffusion barrier of 0.12 eV.

*Keywords: Hydrides, hydrogen storage, ammonia synthesis, hydride ion conduction*

# The synergistic effect of Ni and Pd for Boosting the hydrogen storage performance of $MgH_2$

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## Abstract

$MgH_2$, as a typical solid-state hydrogen storage material, has attracted extensive interest from researchers. However, the high desorption temperature, slow kinetics, and poor cycle stability limit its application and development. At present, adding catalyst is one of the most effective strategies for solving these challenges, among which the transition metal catalyst is the most representative. Recent studies have demonstrated that the synergy between metallic elements frequently exhibits better catalytic effects than a single catalyst. Such a synergistic effect may result in fresh enhancements to the hydrogen storage performance of $MgH_2$.

Herein, we provide a highly efficient metal-based addition constituted of lower-active elements of Pd for enhancing the hydrogen storage performance of $MgH_2$. Due to the synergistic effect between Ni and Pd, the $MgH_2$ with $Ni(acac)_2$ and $Pd(acac)_2$ added exhibited faster dehydrogenation kinetics and higher hydrogen storage capacity than the $MgH_2$ catalyzed by mono metallic Pd additions. The $MgH_2$-Ni-Pd composite can release about 6.9 wt.% of $H_2$ within about 10 min, whereas the $MgH_2$-Pd composite can only desorb approximately 5.0 wt.% of $H_2$ in the same period. This means that Ni can enhance the catalytic activity of Pd element. Overall, this work indicates that using a synergistic effect is an effective way to design efficient catalysts for improving the hydrogen storage performance of $MgH_2$.

*Keywords: Hydrogen storage; Magnesium hydride; Catalyst; kinetics; Salt of acetylacetonate*

# Surface structures and hydrogenation properties of Ti-Pd alloys immersed in hydrogen peroxide.

**Ryota Kondo**[1], Yoshihiro Myokai[2], Yasushi Obora[3], Hiroyuki H. Takeshita[4]

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## Abstract

Ti-xPd (x = 0-1mol%) alloys were shown to have low-valence Pd precipitation on the surface due to the formation of a spontaneous oxide film, which led to fast hydrogen absorption and could be effectively used for organic reactions using the surface Pd (R. Kondo, *Materials Transactions*, 2018, 1911.). However, Pd alloying components remain in the internal region. Therefore, active Pd utilisation is required. In this study, surface treatment by oxidation of Ti-Pd using $H_2O_2$ as oxidant was carried out. The Pd concentration on the alloy surface increased, resulting in fast hydrogen absorption into the Ti phase. The results also supported that the Ti oxide delayed the access of hydrogen to the metallic phase; the immersion of the Ti-1Pd alloys in $H_2O_2$ also resulted in the fast completion of gas emission due to the decomposition of $H_2O_2$. This result correlates with the finding that the amount of Ti dissolved in $H_2O_2$ decreases with increasing Pd concentration in Ti-Pd alloys. On the other hand, the oxidising solvent $H_2O_2$ also had the effect of increasing the thickness of the Ti surface oxide layer; the structure of the Ti-Pd alloys immersed in $H_2O_2$ solution showed an outer oxide phase towards the inner metallic phase, where Pd precipitates, Ti oxides form and the metallic phase are formed. However, the supply of H to the metallic phase was accelerated by the Pd on the surface and retarded by the oxide layer. Model experiments with chip-like samples supported the result that Ti hydrogenation was achieved by the effect of Pd on the surface.

*Keywords: Ti, Hydrogen storage, surface oxide, Pd, surface treatment*

# Disproportionation of $Ti_4Ni_2O_x$ (x=0～1) in $H_2$ atmosphere

**Yuki Kashiyama[1],** Toki Asai[2], Ryota Kondo[3] and Hiroyuki T. Takeshita[4]

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## Abstract

$Ti_2NiO_{0.5}$ ($Ti_4Ni_2O$), an oxygen solid solution of $Ti_2Ni$, can reversibly absorb and desorb hydrogen under ambient conditions such as 293 K and 0.1~1 MPa of $H_2$, in spite that the hydrogen desorption of $Ti_2Ni$ requires much higher temperature. It is known for $Ti_2Ni$ that the disproportionation, which causes its irreversible decomposition into $TiH_2$ and $TiNi_3$, leads to the decrease in the cycle durability of hydrogenation and dehydrogenation. However, there is little information about the disproportionation of $Ti_4Ni_2O$. In this study, it is investigated by ab initio DFT calculations and experiments whether $Ti_4Ni_2O_x$(x=0~1) could possess the same kind of disproportionation as $Ti_2Ni$. The theoretical calculation results suggested that $Ti_4Ni_2O$ can undergo disproportionation which causes its irreversible decomposition into $TiO_y$(y=0~0.50), $TiH_2$ and $TiNi_3$. On the other hand, experimental results at 673 K in 5.0 MPa $H_2$ atmosphere for 80 ks exhibited that disproportionation was confirmed only for $Ti_2Ni$. The results suggest that, although the disproportionation can occur thermodynamically, $Ti_4Ni_2O_x$ is at least kinetically resistant to disproportionation.

*Keywords: hydrogen storage materials, $Ti_4Ni_2O$, $Ti_2Ni$, disproportionation*

# $LaNi_5$ Metal Hydride as a Catalyst for Liquid Organic Hydrogen Carrier

**Sung Ju Han**[1, 2], Hyangsoo Jeong[3, *], Heung Nam Han[4, *], Jin-Yoo Suh[5, *]

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**Abstract**

The need for clean energy sources has led to the emergence of hydrogen energy as a promising alternative. Hydrogen storage methods, such as metal hydrides and Liquid Organic Hydrogen Carriers (LOHC), have garnered significant attention. This study focuses on the use of $LaNi_5$ metal hydride as a catalyst for toluene LOHC. The main objectives of this research were to investigate the feasibility of using $LaNi_5$ as a catalyst for toluene LOHC, and to study the hydrogenation and dehydrogenation behaviour of $LaNi_5$ under liquid.

The catalysis was conducted by introducing toluene into a reactor containing activated $LaNi_5$, and elevating the hydrogen pressure, and temperature. The resulting liquid was analysed with Nuclear Magnetic Resonance (NMR), and analysis revealed an impressive conversion rate of almost 100 % from toluene to methylcyclohexane, indicating the efficiency of the $LaNi_5$ catalyst. Also, from the experimental results, it was shown that $LaNi_5$ can be hydrogenated and dehydrogenated even when immersed in liquid.

The utilization of metal hydrides as catalysts offers distinct advantages, including their cost-effectiveness compared to noble catalysts. Additionally, when the LOHC container is depleted of LOHC, it can serve as a metal hydride hydrogen storage tank. These findings contribute to the understanding and potential applications of $LaNi_5$ as a catalyst for hydrogen storage and LOHC systems.

*Keywords: metal hydride; $LaNi_5$; hydrogen storage; LOHC; catalyst*

# Technical **Oral Session _ Session 5**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 5 (H5)** **14:00 - 15:25, Nov. 21**

**Chair :** To be announced 303B, 3F

14:00-14:20 **I-H1083** **[Invited] Magnetic-field modulation of topological electronic state and emergent magneto-transport in a magnetic Weyl semimetal**
Enke Liu (Chinese Academy of Sciences, China)

14:20-14:40 **I-H1072** **[Invited] Field-free magnetization switching driven by perpendicular spin-polarization at NiO/Pt interface**
Xiaoguang Xu (Beijing University of Science and Technology, China)

14:40-14:55 **O-H1086** **Vegard's law deviating Ti2(SnxAl1–x)C solid solution with enhanced properties**
Zhihua Tian (Southeast University, China)

14:55-15:10 **O-H0969** **Magnetocaloric composites with anisotropic structure prepared in an external magnetic field**
Yanyan Shao (Nanjing University of Science And Technology, China)

15:10-15:25 **O-H0600** **Exploration of Oxygen Doping in GeTe for Phase Change Memory Application**
Shin Young Kang (Tohoku University, Japan)

# Magnetic-field modulation of topological electronic state and emergent magneto-transport in a magnetic Weyl semimetal

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## Abstract

The modulation of topological electronic state by an external magnetic field is highly desired for condensed-matter physics. Schemes to achieve this have been proposed theoretically, but few can be realized experimentally. Here, combining transverse transport, theoretical calculations, and scanning tunnelling microscopy/spectroscopy (STM/S) investigations, we provide an observation that the topological electronic state, accompanied by an emergent magneto-transport phenomenon, was modulated by applying magnetic field through induced non-collinear magnetism in the magnetic Weyl semimetal $EuB_6$. A giant unconventional anomalous Hall effect (UAHE) is found during the magnetization re-orientation from easy axes to hard ones in magnetic field, with a UAHE peak around the low field of 5 kOe. Under the reasonable spin-canting effect, the folding of the topological anti-crossing bands occurs, generating a strong Berry curvature that accounts for the observed UAHE. Field-dependent STM/S reveals a highly synchronous evolution of electronic density of states, with a dI/dV peak around the same field of 5 kOe, which provides evidence to the folded bands and excited UAHE by external magnetic fields. This finding elucidates the connection between the real-space non-collinear magnetism and the ***k***-space topological electronic state and establishes a novel manner to engineer the magneto-transport behaviours of correlated electrons for future topological spintronics.

*Keywords: Magnetic Weyl semimetal, magnetic field modulation, Berry curvature, spin canting, STM/S*

# Field-free magnetization switching driven by perpendicular spin-polarization at NiO/Pt interface

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**Abstract**

Manipulating spin polarization orientation is challenging but crucial for field-free spintronic devices. Although such manipulation has been demonstrated in a limited number of antiferromagnetic metal-based systems, the inevitable shunting effects from the metallic layer can reduce the overall device efficiency. In this study, we propose an antiferromagnetic insulator-based heterostructure NiO/Ta/Pt/Co/Pt for such spin polarization control without any shunting effect in the antiferromagnetic layer. We show that zero-field magnetization switching can be realized and is related to the out-of-plane component of spin polarization modulated by the NiO/Pt interface. The zero-field magnetization switching ratio can be effectively tuned by the substrates, in which the easy axis of NiO can be manipulated by the tensile or compressive strain from the substrates. Our work demonstrates that the insulating antiferromagnet based heterostructure is a promising platform to enhance the spin-orbital torque efficiency and achieve field-free magnetization switching, thus opening an avenue towards energy-efficient spintronic devices.

*Keywords: Spin-orbit torque, antiferromagnetic insulator, spin-polarization.*

# Vegard's law deviating $Ti_2(Sn_xAl_{1-x})C$ solid solution with enhanced properties

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## Abstract

MAX phases are a series of non-van der Waals ternary layered ceramics with a hexagonal structure, also possessing metal-like properties, such as electrical conductivity and magnetism, making them ideal for extreme environments like high temperatures, corrosion, and irradiation. The achievement of chemical diversity and performance regulation of MAX phases primarily relies on solid solution approaches. However, the reported A-site solid solution is undervalued due to its expected chemical disorder and compliance with Vegard's law, as well as discontinuous composition and poor purity. Herein, we synthesized high-purity $Ti_2(Sn_xAl_{1-x})C$ ($x$ = 0–1) solid solution by the feasible pressureless sintering, enabling us to investigate their property evolution upon the A-site composition. The formation mechanism of $Ti_2(Sn_xAl_{1-x})C$ was revealed by thermal analysis, and crystal parameters were determined by Rietveld refinement of X-ray diffraction (XRD). The lattice constant ($a$) adheres to Vegard's law, while the lattice constant ($c$) and internal free parameter ($z_M$) have noticeable deviations from the law, which is caused by the significant nonlinear distortion of $Ti_6C$ octahedron as Al atoms are substituted by Sn atoms. Also, the deviation also results in nonlinear changes in their physicochemical properties, which means that the solid solution often exhibits better performance than end members, such as hardness, electrical conductivity, and corrosion resistance. This work offers insights into the deviation from Vegard's law observed in the A-site solid solution and indicates that the solid solution with enhanced performance may be obtained by tuning the A-site composition.

*Keywords: MAX phase; $Ti_2(Sn_xAl_{1-x})C$; Vegard's law; high purity; properties*

[1] **Z.H. Tian**, P.G. Zhang*, Z.M. Sun*, Vegard's law deviating $Ti_2(Sn_xAl_{1-x})C$ solid solution with enhanced properties, Journal of Advanced Ceramics, 2023, online first. https://doi.org/10.26599/JAC.2023.9220779
[2] **Z.H. Tian**, P.G. Zhang*, Z.M. Sun*, et al. Synthesis of $Ti_2(In_xAl_{1-x})C$ ($x$=0–1) solid solutions with high-purity and their properties, Journal of the European Ceramic Society, 2023, 43: 5915.
[3] **Z.H. Tian**, P.G. Zhang*, Z.M. Sun*, et al. Synthesis of $Ti_3(Sn_xAl_{1-x})C_2$ solid solutions over the whole composition, Journal of Alloys and Compounds, 2022, 894: 162429.

# Magnetocaloric composites with anisotropic structure prepared in an external magnetic field

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Active magnetic regenerator (AMR) cycle has been utilized to enlarge temperature change range of magnetic refrigerator. The efficiency of heat exchange between the refrigerant and the fluid is crucial, and anisotropic heat exchange perpendicular to the fluid direction is desirable. In this study, a mixture of La-Fe-Si powder and polymer fluid was placed into a mold and subjected to an external magnetic field. In a magnetostatic field, the sample experienced a vertical magnetic force, as depicted in Figure 1a. By rotating the sample, it can be considered as being subjected to a rotating magnetic field (Figure 1b). As shown of scanning electron microscope (SEM) images, the random distribution of samples in magnetostatic field (Figure 1c) can be observed. By the contrast, the magnetic La-Fe-Si powder moved into an array-like configuration for the case of rotating magnetic field, presenting an anisotropic distribution of the La-Fe-Si particle (Figure 1d). Corresponding three-dimensional distribution of the phases were also shown here. The thermal diffusivity of samples prepared in the magnetic field was investigated and depicted in Figure 2. It is apparent that the difference in thermal diffusivity between different directions in a rotating magnetic field is much larger than that in a magnetostatic field, thereby confirming the anisotropic thermal property. It is important to note that the relatively low thermal diffusivity is due to the low thermal properties of the polymer used. Further research in phase selection can offer promising opportunities for enhancing the thermal properties and overall performance of the magnetic refrigerator system.

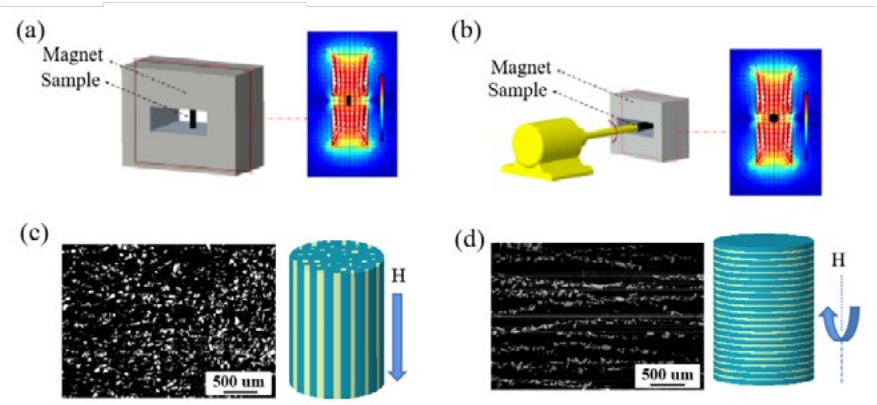



Figure 1. Diagrams of magnetostatic (a) and rotating magnetic field (b), with distribution of magnetic induction intensity. SEM images of samples prepared at magnetostatic (c) and rotating magnetic field (d), the corresponding demonstration were also shown.

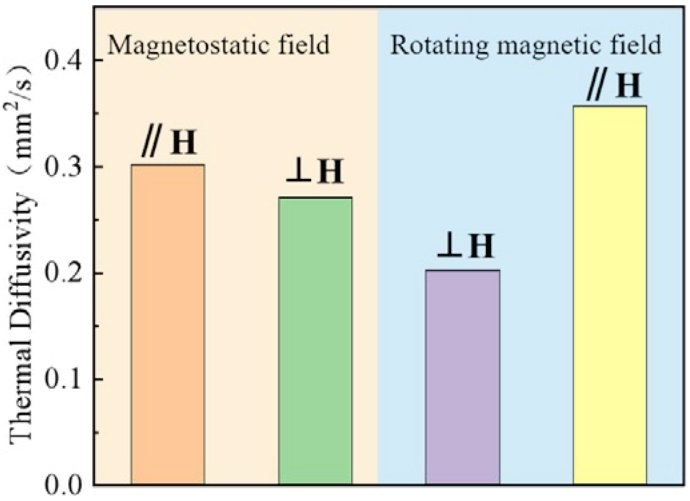



Figure 2. Thermal diffusivity of samples prepared at magnetostatic and rotating magnetic field.

# Exploration of Oxygen Doping in GeTe for Phase Change Memory Application

**Shinyoung Kang[1],** Kota Jojima[1], Mihyeon Kim[1], Shuang Yi [2], Daisuke Ando[1], Yuji Sutou[1,2]

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## Abstract

Phase change memory (PCM) is one of the keys enabling memory technologies for next-generation non-volatile memory device applications owing to its fast erasing/writing speeds (50 ns/10 ns), and good scalability [1]. However, the high-power consumption of PCM devices caused by the high switching current from a high resistive state (RESET) to a low resistive state (SET) is a critical obstacle to be resolved before widespread commercialization can be realized [1]. In this investigation, oxygen doping is introduced to boost the endurance and the data retention of GeTe without sacrificing power consumption. Fig. 1(a) shows the results of resistance-temperature measurements, which are fulfilled in an Ar to characterize resistance films as a function of temperature. The doping oxygen increases the phase transition temperature of films and improves the thermal stability to achieve better data retention. The optical bandgap of films is shown in Fig. 1(b). According to the fitting curves, the optical bandgap of the amorphous state was calculated to be 0.77 eV for GeTe, and 1.18 eV for oxygen 0.9 sccm. The PCM devices based on O-doped GeTe were fabricated by focus-ion beam drilling (FIB). As shown in Fig 1 (c), the PCM device exhibited a threshold switching from the amorphous to the crystalline phase. It reveals a good electrical performance of O-doped GeTe which high/low resistance ratio is over $10^4$ Ω. These results show that the O-doped GeTe material can be a potential candidate for PCM applications.

*Keywords: germanium telluride, phase change memory, high endurance, doping*

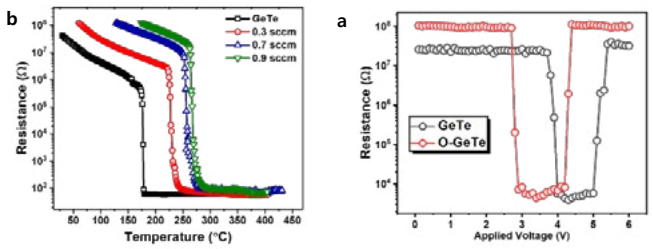



**Fig. 1** (a) Resistance of GeTe, O-doped GeTe films as a function of the temperature. (b) R-V performance of the GeTe and O-doped GeTe cell.

## Reference

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## Acknowledgements

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# Technical **Oral Session _ Session 5**

## **Symposium I :** Biomaterials and Soft Materials and their Application

**Biomaterials and Soft Materials and their Application 5 (I5)** **14:00 - 15:50, Nov. 21**

**Chair :** Yufeng Zheng (Peking University), Nikolay Redko (Moscow State University) 400, 4F

14:00-14:30 **K-I1091** **[Keynote] Structure, mechanical and corrosion properties bioresorbable magnesium alloys of Mg-Zn-Ga and Mg-Zn-Ca-Mn systems for medical purpose**
Alexander Komissarov (Moscow State University, Russia)

14:30-14:50 **I-I0721** **[Invited] Development of Mg-Zn alloys with low impurities by vacuum distillation and extrusion for excellent corrosion resistance**
Kyosuke UEDA (Tohoku University, Japan)

14:50-15:10 **I-I1157** **[Invited] Bioelectrochemical interfaces: Bridging digital and biological systems**
Jimin Park (Korea Advanced Institute of Science And Technology, Korea)

15:10-15:30 **I-I0358** **[Invited] Mg alloys and processes for temporary biodegradable implants in orthopedic and vascular applications**
Joung Sik Suh (Korea Institute of Materials Science, Korea)

15:30-15:50 **I-I0945** **[Invited] Surface-Roughness-Induced Plasticity in a Biodegradable Zn Alloy**
Luning Wang (University of Science and Technology Beijing, China)

# Structure, mechanical and corrosion properties bioresorbable magnesium alloys of Mg-Zn-Ga and Mg-Zn-Ca-Mn systems for medical purpose

**Alexander Komissarov**[1], Viacheslav Bazhenov[2], Stanislav Rogachev[3], Anna Li[4], Denis Ten[5], Nikolay Redko[6], Alexey Drobyshev[7], Kwang Seon Shin[8]

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Five alloys of the Mg-Zn-Ga system were developed: MgZn4Ga4; MgZn4Ga4Y0.5; MgZn6.5Ga2; MgZn4Ga2 and MgZn2Ga2. Four alloys of the Mg-Zn-Ca-Mn system were developed: MgZn2Ca0.7; MgZn4Ca0.7; MgZn2Mn1Ca0.7 and MgZn4Mn1Ca0.7. To improve the mechanical and corrosion properties, the alloys were deformed by hot extrusion. For all alloys, the microstructure was studied, the mechanical properties were determined in the longitudinal and transverse directions of extrusion.

Additionally, for all alloys, the corrosion rate was determined from the evolution of hydrogen in Hank's solution. It was found that the corrosion rate in Hank's solution depends on the chemical composition of the alloys. With an increase in the content of zinc and gallium in alloys, the corrosion rate increases. Thus, after extrusion at a temperature of 150 °C, the MgZn2Ga2 alloy has a corrosion rate of 0.2 mm/g required for medical devices. This alloy additionally has a therapeutic effect due to the presence of gallium in it. The MgZn2Ca0.7Mn1 alloy after extrusion at a temperature of 300 °C has a corrosion rate of 0.5 mm/g required for medical devices.

According to the results of the cytotoxicity study of alloys of the Mg-Zn-Ga and Mg-Zn-Ca-Mn systems, it was found that the MgZn2Ga2 alloy extruded at 150 °C did not show significant cytotoxicity towards MG63 cells according to ISO 10993-5. According to the results of the study of cytotoxicity of alloys of the Mg-Zn-Ca-Mn system, it was found that the MgZn2Ca0.7Mn1 alloy extruded at 300 ° C showed moderate cytotoxicity towards MG63 cells according to ISO 10993-5.

*Keywords: Magnesium alloys, structure, properties, cytotoxicity*

# Development of Mg-Zn alloys with low impurities by vacuum distillation and extrusion for excellent corrosion resistance

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**Abstract**

Mg and its alloys are expected to be applied to bioresorbable bone plates because it is an essential element that is soluble *in vivo*. However, the dissolution of commercially pure (CP) Mg is too rapid *in vivo* to heal bone fractures. Intermetallic inclusions originating from impurities, such as Fe, are known to cause galvanic corrosion, resulting in reduced corrosion resistance. Thus, the removal of impurities from Mg is an effective method for suppressing Mg dissolution.

This study focused on vacuum distillation, which can achieve highly pure Mg and introduce Zn because of its high vapor pressure. Commercial Mg-Zn alloys were vacuum-distilled, and highly pure Mg billets with various Zn concentrations were obtained. The highly pure Mg-Zn alloy plates were prepared by extrusion without melting, and no contamination was observed.

After 6 d of immersion in simulated body fluids, the CP Mg plates were fractured into pieces because of the inhomogeneous dissolution from the intermetallic inclusions. In contrast, the highly pure Mg-Zn alloy plates dissolved homogeneously, and calcium phosphate layers formed on the surface. The plate mass loss was successfully evaluated by removing only the calcium phosphate layer using chromic acid treatment. A Zn content of up to 0.9 mass% reduced the plate mass loss and suppressed dissolution. In contrast, at a Zn content of 3 mass%, dissolution was accelerated owing to Mg-Zn intermetallic formation.

*Keywords: Highly pure Mg, dissolution behavior, immersion test, bioresorbability.*

# Bioelectrochemical interfaces: Bridging digital and biological systems

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## Abstract

During the last few decades, electronic devices for recording and modulating electrical signals in biological systems have been applied to treat diseases and study biological systems. To further advance the communication between digital and biological systems, however, we need to consider biochemical signals, which affect the physiology and pathology of biological systems in a complex way.

In this talk, I will introduce bioelectrochemical interfaces that can modulate biochemical signals with digital inputs. Central to these interfaces is the use of biomimetic nanocatalysts for the electrochemical generation of chemical signals [1-2]. I have demonstrated that these interfaces can be integrated into a wide range of biomaterials, including orthopedic implants and cardiovascular stents, to control cellular signaling [3]. Recently, I extended this approach to develop neural probes capable of electrochemically producing gaseous neurotransmitters in the brain [4-5]. These probes enable the study of how these chemical signals affect neural signaling and animal behavior. I envision that my research in bioelectrochemical interfaces will advance our understanding and control over biological systems.

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# Mg alloys and processes for temporary biodegradable implants in orthopedic and vascular applications

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## Abstract

Magnesium (Mg) alloys are receiving increasing attention as potential metallic biomaterials for temporary biodegradable implants in orthopedic and vascular applications due to their mechanical, electrochemical and biological properties. However, Mg scaffolds still have some difficulties such as high degradation rate, low mechanical properties, difficult fabrication method and some biocompatibility issues. For load-bearing implants, biodegradable Mg alloys require a sufficiently slow degradation rate and a high compressive strength above the level of compact bone to support bone regeneration. In particular, the plasticity is crucial for biodegradable vascular stents to expand with large deformation upon implantation after being crimped onto a balloon catheter. Alloying and processing are key approaches to improving the comprehensive properties of Mg alloys for biomedical applications.

We introduce basic research results for patient-specific bone scaffolds by applying additive manufacturing (AM) to a new biodegradable Mg alloy. The microstructure, mechanical properties and in vitro corrosion rate of the AM specimens are evaluated and compared with as-cast samples.

For bioresorbable stents, this study investigates the mechanical properties of Mg microtube processed by direct double extrusion, focusing on roundness and dimensional accuracy. The mechanical behavior of as-fabricated Mg microtube is analyzed with respect to changes in microstructure and texture. The improved plasticity of as-extruded microtube can be attributed to grain boundary strengthening and texture weakening.

*Keywords: Magnesium Alloy, Biodegradable Implant, Additive Manufacturing, Microtube, Double Extrusion*

# Surface-Roughness-Induced Plasticity in a Biodegradable Zn Alloy

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## Abstract

Zn-based materials have attracted growing attention as biodegradable metallic materials. Good plasticity is important for processing Zn-based materials into medical implants. It is also critical to functioning of some medical implants, such as balloon-expandable stents. However, it is difficult to increase room-temperature elongation of metallic materials over 100% without sacrificing strength using existing methods. Herein, surface-roughness-induced plasticity (SRIP) is discovered in biodegradable Zn–0.4Mn alloy. Surprisingly, in the good surface range that meets the international standard ISO 6892, reducing surface roughness results in significant increase in plasticity without loss of strength. From unground to 5000# sandpaper ground states, the surface roughness Ra of the alloy decreases from 0.63 to 0.05 μm, while its room temperature elongation increases from 74% to 143%. SRIP is the synergistic result of increased microstructure damage tolerance and decreased surface roughness. It provides a new method for improving the plasticity of biodegradable Zn alloys.

*Keywords: biodegradable Zn; plasticity; surface roughness; strength; microstructure*

# Technical **Oral Session _ Session 5**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 5 (J5)** **14:00 - 15:25, Nov. 21**

**Chair :** Wataru YASHIRO (Tohoku University) 201B, 2F

14:00-14:30 **K-J0755** **[Keynote] Materials Characterisation and Modelling, Critical for the Materials Development Lifecycle**
Natasha Wright (CSIRO, Australia)

14:30-14:50 **I-J0464** **[Invited] A machine-learning assisted optimization approach and microstructure characterization method for laser powder bed fusion**
Xiaopeng Li (University of New South Wales, Australia)

14:50-15:10 **I-J0770** **[Invited] Geological Sequestration of CO2 in Sandstone Formations: Deep Dive into Residual Trapping Mechanisms**
Mohammad Saadatfar (The University of Sydney, Australia)

15:10-15:25 **O-J0676** **Simulation of the blister formation in the electro-galvanized steel**
Sang-Hoon Shin (Pohang University Of Science And Technology, Korea)

# Materials Characterisation and Modelling, Critical for the Materials Development Lifecycle

**Natasha Wright**[1], Sheridan Mayo[1], Roger Mulder[1]

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## Abstract

Materials Characterisation and Modelling are integral to the materials development lifecycle, providing the evidence, data and insights which underpin every step of this complex process. Characterisation of Novel Materials can be a significant challenge due to the complex systems and interfacial interactions of the constituents, which can be at levels ranging from subnano - to micro-scale. Compared with conventional, bulk analyses, the need -to holistically characterise these distributions and interactions has continued to grow in importance within CSIRO. This paper highlights how the combination of multi-scale imaging (including 3D tomography), micro and thin-film X-ray diffraction, spectroscopic and surface analysis techniques (XPS, AFM) has enabled us to holistically characterise several examples of custom engineered novel materials and devices developed by CSIRO's Manufacturing Business Unit.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: Characterisation, Materials and Process modelling, Novel Materials, Materials Development Lifecycle, Additive Manufacturing, X-ray Photo Spectroscopy, Micro CT, Atomic Force Microscopy, Electron Microscopy, Synchrotron, X-ray diffraction*

**A machine-learning assisted optimization approach and microstructure characterization method for laser powder bed fusion**

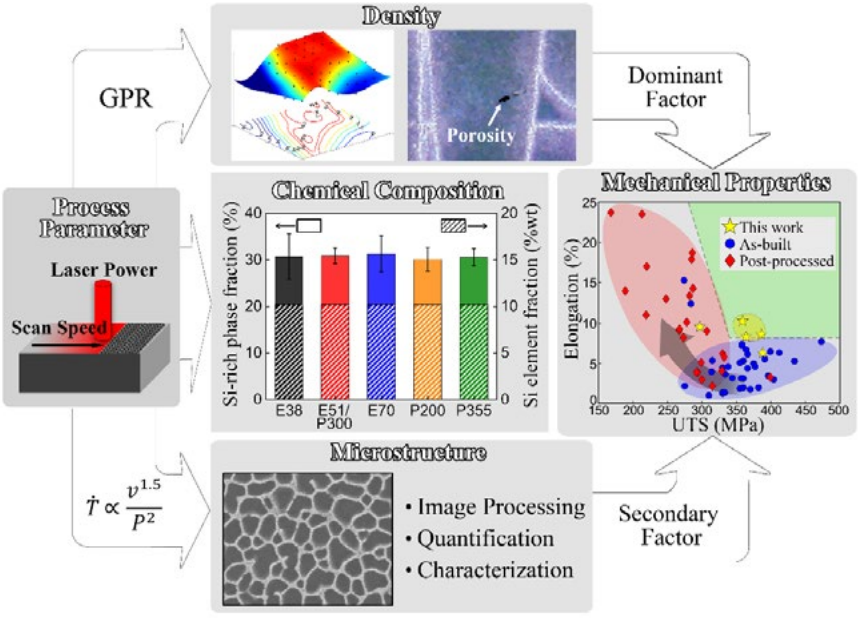
Qian Liu, Hongkun Wu, Moses J. Paul, Peidong He, Zhongxiao Peng, Bernd Gludovatz, Jamie J. Kruzic, Chun H. Wang, Xiaopeng Li

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Laser powder bed fusion (LPBF) technique, as one of the most popular metal additive manufacturing (AM) techniques, has been employed for various materials fabrication due to its excellent advantages (e.g., freedom of design) compared to the traditional fabrication methods. However, a wide range of fabrication process parameters make it difficult to develop materials with this technique because corresponding suitable parameters usually rely on a costly trial-and-error process and a large number of experiments. In this work, we propose a new paradigm of LPBF process optimization for AlSi10Mg alloy based on Gaussian process regression (GPR) and limited experimental data. Our work found a new and much larger optimized LPBF processing window than was reported before for fabricating fully dense LPBF AlSi10Mg samples. More optimized manufacturing parameters make us possible to achieve previously unattainable combinations of desirable mechanical properties (high strength and ductility). Besides, in order to better manipulate the microstructure for desired mechanical properties in LPBF AlSi10Mg alloy, we introduced image processing technique and generated two newly defined morphology indices (i.e., dimensional-scale index $I_d$ and shape index $I_s$) for microstructure characterization based on several key microstructural features obtained from SEM images. This proposed approach enables quick identification of the optimized LPBF processing window and the establishment of process-structure-property relationship for AlSi10Mg, which is believed to be applicable to other widely used metals and alloys or newly designed LPBF materials.

**Keywords:** Additive manufacturing, Gaussian process regression (GPR), Aluminum alloy




*Investigated process-structure-property (PSP) link in Al-Si alloy in LPBF*

# Geological Sequestration of CO2 in Sandstone Formations: Deep Dive into Residual Trapping Mechanisms

**Mohammad Saadatfar[1,2]**, Anna Herring[3], Farshad Daraei Ghadikolaei[4], Ruotong Huang[5]

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## Abstract

Among the practical strategies for atmospheric emission reduction outlined by the Intergovernmental Panel on Climate Change (IPCC), geological storage of $CO_2$ offers immense promise with the potential to significantly impact emission and atmospheric $CO_2$ reduction. Residual trapping of supercritical carbon dioxide ($scCO_2$) plays a substantial role in enhancing the safety and efficacy of geologic sequestration operations.

Recent investigations indicate that cycles of $scCO_2$ and brine injections trigger surface chemistry reactions, enhancing residual entrapment. The results of our recent experiment, analysed through combined X-ray micro-computed tomography and modelling in both 3D and 4D, aim to further elucidate the specifics of this alteration mechanism. In our in-situ experimental cycles, multiple $scCO_2$ injections were carried out, with varied injection flow rates. Our observations indicate consistent saturation profiles near the lower permeability layer, while downstream $scCO_2$ saturation profiles transform and generally increase with successive injections. 3D/4D microstructural analysis of the $scCO_2$ phase revealed a growing presence of surfaces with high contact angles, suggesting a decrease in water-wetting as the experiment progressed.

These findings propose that surface chemistry alterations transpire during drainage injections and potentially during imbibition. This effect is primarily discernible within the high permeability region of the core. In the low permeability region, flow patterns are predominantly dictated by capillary heterogeneity, with no significant effects of wettability alteration. Our findings provide fresh insights into the specific conditions under which wettability alteration induces shifts in $scCO_2$ flow and trapping.

*Keywords: X-ray micro-tomography, Geologic $CO_2$ sequestration, Capillary trapping, Permeability*

# Simulation of the blister formation in the electro-galvanized steel

**Sang-Hoon Shin**[1], Bong-Hoon Chung [2], Yong-Gyun Jeong[3], Yoon-Uk Heo[1*]

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## Abstract

The formation behavior of the blister in electro-galvanized steel was studied by simulating the zinc-deposited specimen in the laboratory. The micro-crack and delamination were artificially introduced at the interface between the zinc layer and steel substrate. The steel surface is mechanically polished or contaminated with oil to introduce cracks or delamination before electro-galvanizing process.

Hydrogen charging was applied in the solution (NaCl(3%)+$NH_4SCN$(3g/L)) under the bias condition of 20 mA/$cm^2$. Blister formation was identified on the surface of the electro-galvanized steel after the hydrogen charging. The expansion of the interface crack was identified in the cross-section of a blister so interface crack is the initiation site of the blister. Through TOF-SIMS experiments, hydrogen ion and methane ion were measured inside the blisters. Therefore, the blister was generated by pressure of hydrogen and methane gas.

Further hydrogen charging and thermal desorption test reveal the role of hydrogen diffusion in the steel substrate and zinc layer on the blister formation. The baking treatment results in the formation of a blister at the zinc/steel interface under specific conditions. The blister formation mechanism is discussed by the obtained results.

*Keywords: Electro-galvanized steel, Blister, Hydrogen*

# Technical **Oral Session _ Session 5**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 5 (K5)** **14:00 - 15:40, Nov. 21**

**Chair :** Nam Hyun Kang (Pusan National University) Samda Hall B, 3F

14:00-14:20 **I-K0777** **[Invited] Design and Development of Refractory High-entropy Alloys via An Experimentally Driven High-throughput Approach**
Saryu Fensin (Los Alamos National Laboratory, USA)

14:20-14:40 **I-K0633** **[Invited] Systematic investigation regarding solid-solution strengthening in Refractory High Entropy Alloys**
Gi An Song (Kongju National University, Korea)

14:40-15:00 **I-K0268** **[Invited] Mechanical properties of a high entropy bcc TiZrNbHfTa refectory alloy**
Masaki Tanaka (Kyushu University, Japan)

15:00-15:20 **I-K0978** **[Invited] Overcoming oxygen embrittlement of refractory high-entropy alloy via grain boundary engineering**
Yuan WU (University of Science and Technology Beijing, China)

15:20-15:40 **I-K0111** **[Invited] First-principles study on mechanical properties and dislocation core in BCC refractory high-entropy alloys**
Tomohito Tsuru (JAEA, Japan)

**Design and Development of Refractory High-entropy Alloys via An Experimentally Driven High-throughput Approach**

Chanho Lee, Dongyue Xie, Benjamin Kyle Derby, Jon Kevin Baldwin, Christopher Tandoc, Osman Ei Atwani, Yong-Jie Hu, Nan Li, and Saryu J. Fensin

High-entropy alloy (HEA) design strategies have been limited to theoretical/computational approaches due to their compositional complexity and extremely large compositional parameter space. In this work, we developed an experimentally driven, high-throughput, HEA design approach using a physical vapor deposition (PVD) technique and coupled it with nanomechanical testing to accelerate material design for structural applications. The PVD technique enabled the formation of a compositional gradient across a thin-film sample. Specifically, a 10 cm wafer was used to manufacture a continuous set of 80 HEA compositions within the Nb-Ti-V-Zr family using a single deposition cycle. By applying the solid-solution strengthening theory and developed machine-learning approaches, the strength and ductility of these HEA compositions were quantitatively determined/predicted and then experimentally verified by nano-indentation hardness test. Consequently, 7 refractory HEA compositions were successfully down-selected based on optimized strength and ductility predictions.

# Systematic investigation regarding solid-solution strengthening in Refractory High Entropy Alloys

**Kangjin Lee[1], Yunjong Jung[1], Junhee Han[2], Chanho Lee[3], Peter K. Liaw[4], Gian Song[1*]**

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Refractory High-Entropy Alloys (RHEAs) have attracted significant attention, due to their outstanding properties and microstructural stability at elevated temperatures. In many RHEAs, the solid-solution strengthening mechanism plays a main role in their excellent mechanical properties. The solid-solution strengthening in HEAs is known to be affected by the lattice and shear modulus distortion factors, which are closely related with lattice misfit, bonding energy misfit and different crystal structure among alloying elements. Especially, it has been reported that the yield strength of many RHEAs with single-phase BCC structure is enhanced by maximizing the lattice distortion factor.
In this study, to establish the concrete relationship between the lattice distortion factor and yield strength of the RHEAs, we attempted to validate the effect of the lattice distortion factors on solid-solution strengthening effect in refractory alloys by systematic alloy design. Specifically, we fabricated a number of equi-atomic refractory alloys, forming BCC single solid-solution phase. Their microstructure evolution and mechanical properties were systematically investigated using neutron diffraction, scanning electron microscopy, electron backscatter diffraction and universal testing machine

Key words : High Entropy alloys; Microstructure; Mechanical Properties

# Mechanical properties of a high entropy bcc TiZrNbHfTa refectory alloy

**Masaki Tanaka**[1]

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## Abstract

The temperature dependence of the yield stress, effective stress, activation volume and activation enthalpy in a polycrystalline bcc high entropy TiZrNbHfTa refractory alloy has been investigated by tensile tests at 77 – 750 K. The Peierls stress was estimated to be 580 MPa by extrapolating the effective shear stress to 0 K. The activation enthalpy below 260 K corresponds to that of other bcc crystals with high Peierls potentials, suggesting kink-pair nucleation is the controlling mechanism of the dislocation glide in this temperature range. Meanwhile, the activation enthalpy above 260 K deviated from the trendline, indicating the changes in the dislocation glide from the kink-pair nucleation to the other one. The slip properties of TiZrNbHfTa were also evaluated by micrometre cantilever bending tests in order to understand the mechanism behind the fact that extreme straight slip bands are seen on the specimen surface after plastic deformation, as it suggests that the cross-slip should be suppressed. The ψ-χ relationship indicated, instead, that slip planes are not persisted on the specific crystallographic planes. Detailed observations with atomic force microscopy revealed anomalously frequent cross slip on a sub-micron length scale, explaining the extreme straight slip bands seen on the surface after plastic deformation.

*Keywords: bcc, slip, dislocation, plastic deformation, cross-slip*

# Overcoming oxygen embrittlement of refractory high-entropy alloy via grain boundary engineering

**Yuan Wu***, Xianzhen Wang, Zhengqi Wang, Xiongjun Liu, Hui Wang, Suihe Jiang, Zhaoping Lu

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**Abstract**

Refractory high-entropy alloys (RHEAs), particularly NbMoTaW RHEAs, exhibit outstanding softening resistance and thermal stability at ultra-high temperatures, but suffer from room-temperature brittleness, which severely limits their processability and thus practical application. In this study, we successfully achieved large plasticity of >10%, along with high strength of >1750 MPa in the NbMoTaW RHEAs via grain boundary engineering with the addition of either metalloid B or C. It was revealed that the room-temperature brittleness of the as-cast NbMoTaW RHEA originates from the grain-boundary segregation of the oxygen contaminant which weakens grain-boundary cohesion. The doped small-sized metalloids preferentially replace oxygen at grain boundaries and promote stronger electronic interaction with the host metals, which effectively alleviates the grain boundary brittleness and changes the fracture morphology from intergranular fracture to transgranular fracture.

*Keywords: refractory high-entropy alloy, grain boundary engineering, mechanical properties, ductilization*

# First-principles study on mechanical properties and dislocation core in BCC refractory high-entropy alloys

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## Abstract

Refractory body-centered cubic (BCC) high-entropy alloys (HEAs) have excellent mechanical properties and their features differ significantly depending on constituent elements. For example, BCC-HEAs containing specific elements show an excellent balance between high strength and elongation and unique slip behavior. Therefore, it is essential to understand the atomic-level depiction of defect structures considering the effects of the constituent elements to elucidate the origin of the unique mechanical properties of HEA. Especially, a detailed exploration of dislocation core structure and motion should be the key to identifying the mechanical properties.
In the present study, we focused on two BCC-HEAs with different features and chose VNbMoTaW and TiZrNbHfTa as widely-discussed alloy systems in the community. We expected that the origin of the difference in mechanical properties was caused by the local lattice distortion, elastic properties, and short-ranged order (SRO) formation, which should be derived from the existence of the group IV elements with a sufficient concentration. We investigate the differences of these properties and the dislocation core features between two BCC-HEAs using the first-principles calculations. As a result, the mean square displacement of TiZrNbHfTa was quite large. This significant lattice distortion originates from the group IV elements, but the SRO formation does not influence the value. Furthermore, the dislocation core of TiZrNbHfTa tends to expand widely, which is totally different from most conventional BCC metals and alloys. The unique core structure and slip behavior of TiZrNbHfTa are also caused by highly concentrated group IV elements.

*Keywords: BCC high-entropy alloys, lattice distortion, dislocation core, first-principles calculations*

# Technical **Oral Session _ Session 5**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 5 (L5)** **14:00 - 15:15, Nov. 21**

Chair : Caroline Sunyong Lee (Hanyang University), Yoshimi Watanabe (Nagoya Institute of Technology) 202B, 2F

14:00-14:30 **K-L0310** **[Keynote] The coming direction of functionally graded materials**
Yoshikazu Shinohara (NIMS, Japan)

14:30-14:45 **O-L0984** **Impact of post-treatment on the microstr uctural behaviour of a Co-based alloy coating developed on Inconel-718 using HVOF technique.**
AVEEK MOHANTY (Indian Institute of Technology Madras, India)

14:45-15:00 **O-L1043** **Modelling SiC heating supports based on microstructural features**
JaeHyung Cho (Korea Institute of Materials Science, Korea)

15:00-15:15 **O-L0393** **Metal-phenolic networks doped all-polybenzoxazine superhydrophobic coatings to boost corrosion and biofouling resistance via integrated design**
Xiangkang Cao (Huazhong University of Science and Technology, China)

# The coming direction of functionally graded materials

**Yoshikazu Shinohara**

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## Abstract

Functionally graded materials (FGMs) were basically defined as materials of which functions change gradually or stepwise inside the materials. Typical ones are heat resistant materials of which composition changes from metal at one side to ceramics at another side. Recently multifunctional materials such as composite materials and coated materials are included in FGMs. The basic concept has been shifted from functional gradient to functional allocation in materials. FGMs were a part of the material field of composite materials originally, and is not clear in difference from composite materials. The present stage of FGMs and the coming direction of FGMs will be presented.

*Keywords: functionally graded materials, FGMs, multifunction, composite materials.*

# Impact of post-treatment on the microstructural behaviour of a Co-based alloy coating developed on Inconel-718 using HVOF technique.

**Aveek Mohanty**[1], S.K Panigrahi[2]

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## Abstract

Ni-based superalloys find extensive applications across various fields, including nuclear, defence, marine and aerospace. However, when exposed to such demanding environments, these components are susceptible to hot corrosion resulting from combined chemical reactions such as sulfidation-oxidation and chlorination. Consequently, surface enhancement emerges as a promising approach to mitigate premature failure of superalloy components in these harsh and aggressive environments. In recent years, High Velocity Oxy Fuel (HVOF) has shown significant advancements among the range of thermal spray techniques employed for depositing protective coatings. HVOF has proven to be a highly versatile technology, offering a reliable and cost-effective solution for numerous industrial applications. The applications of high-energy sources (lasers, electron beams) in post heat-treatments of thermally sprayed protective coatings is a prevalent method to achieve microstructure homogenization through remelting and solidification. However, these processes often induce defects like rapid solidification, thermal distortion, and interfacial cracks in coated samples. To address these limitations, microwave hybrid-heating emerges as a potential solution.
In present work, a protective coating of Co-based alloy powder was developed on Inconel-718 substrate using HVOF process. The as-sprayed (HVOF) coating is heat treated using a domestic microwave. Microstructural characterization of as sprayed and heat-treated coating was done on the clad cross sections using FESEM, EDS and XRD. Porosity and surface roughness were also measured. The microstructural observations of microwave treated clad indicated a good metallurgical bonding with the substrate and revealed no visible interfacial cracking due to homogenization of coating structure.

**Keywords:** Ni-based superalloy, HVOF, Post heat-treatment, Microwave hybrid heating

# Modelling SiC heating supports based on microstructural features

**JaeHyung Cho[1],** Choi Joon-hwan[1], Jeong Ho-jin[1]

[1] Korea Institute of Materials Science, 797, Changwon-daero, Seongsan-gu, Changwon-si, Gyeongsangnam-do, 51508, Korea (12-point Times New Roman, left-aligned)
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**Abstract**

SiC heating elements fabricated by extrusion and sintering consisted of multi-phases of SiC, Si and porosities. Based EBSD/EDS microscopy, microstructural features including volume fraction and shape of each phase were obtained and three-dimensional modelling were constructed. In order to apply electric current flow for Joule heating, all SiC and Si phases were assumed to be connected together. Multi-physics finite element approaches with Joule heating, conduction, and heat transfer were carried out. Depending on overall volume fraction of each phase, effective material properties of thermal conductivity and electrical conductivity of the porous SiC heating elements were predicted and compared with experiments.

*Keywords: SiC, microstructure, porous materials, modelling and simulation*

# Metal-phenolic networks doped all-polybenzoxazine superhydrophobic coatings to boost corrosion and biofouling resistance via integrated design

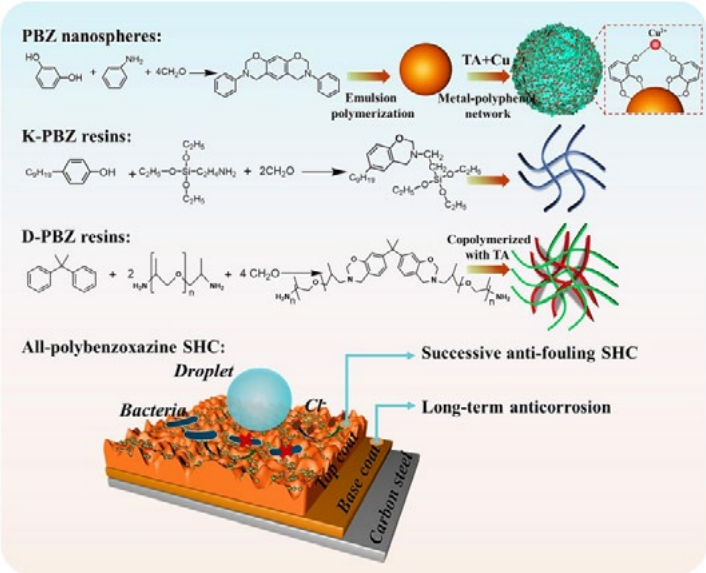
**Xiangkang Cao**[1], Zehua Dong[1,*]

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## Abstract

Polybenzoxazine (PBZ) is a kind of intrinsic low-surface-energy resin, which can be granted versatile properties, such as superhydrophobicity, anti-corrosion, and anti-fouling through flexible monomer design. Herein, we engineered a kind of dual-layered all-PBZ superhydrophobic coating through size-adjustable PBZ nanospheres pre-doped with antibacterial cupric-tannic acid (TA) metal-phenolic networks (Cu-APSHC), in which the 3-aminopropyltriethoxy silane KH550-type PBZ (K-PBZ) resin modified by the Cu-TA@PBZ nanospheres as a superhydrophobic topcoat and the polyetheramine D230-type PBZ (D-PBZ) resin as a primer coat. Chemical and mechanical tests evidenced that the Cu-APSHC features robust non-wettability even upon long-term UV irradiation or saline immersion test, as well as excellent antifouling properties thanks to its durable superhydrophobicity and pH-responsive release of antifouling agent from the topcoat. Besides, salt spray tests (SST) proved that the Cu-APSHC exhibits high corrosion barrier performance (>$10^9$ Ω.cm2 even after 720 h SST). It is therefore envisioned that this work may promote the development of all-polybenzoxazine coatings featured of durable anti-corrosion, anti-fouling, and cost-efficient properties.

*Keywords: polybenzoxazine, superhydrophobic coatings, anti-corrosion, anti-fouling, metal-phenolic networks, monomer design.*




**Scheme 1.** Illustrated preparation of APSHC coating.

# Technical **Oral Session _ Session 5**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 5 (M5)** **14:00 - 15:35, Nov. 21**

**Chair :** Kiet Tieu (University of Wollongong), Eun Ae Choi (Korea Institute of Materials Science) **402, 4F**

14:00-14:30 **K-M1100** **[Keynote] In situ TEM for nanomaterial deformation analysis**
Dmitry Golberg (Queensland University of Technology, Australia)

14:30-14:50 **I-M1175** **[Invited] Evaluation of Mechanical Properties of Irregularly Structured Nanomaterials - Utilization of Nanoindentation Techniques**
Dongyun Lee (Pusan National University, Korea)

14:50-15:05 **O-M1096** **Research of Novel Graphene-Reinforced CuW Electrical Contacts for High Voltage Circuit Breaker**
Yi Ding (State Grid Smart Grid Research Institute Co. Ltd., China)

15:05-15:20 **O-M0692** **Exploring the Influences of Combined Pre-straining and Hydrogenation on the Nanomechanical Behavior of Selectively Laser Melted High-Entropy Alloy**
Zhe Gao (Hanyang University, Korea)

15:20-15:35 **O-M0067** **Antiferromagnetic nanosheet VSxO2-x for microwave absorption in high and low band by adjusting**
Zihan Jiang (Northeastern University-shenyang, China)

# *In situ* TEM for nanomaterial deformation analysis

**Dmitri V. Golberg**[1,2]

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## Abstract

Compression, bending and tensile deformations of diverse inorganic nanomaterials, *e.g.*, nanotubes, nanowires, nanoparticles, and two-dimensional sheets has been realized and in detail studied inside a high-resolution transmission electron microscope column (HRTEM) using dedicated *in situ* TEM holders equipped with piezo motors for nanostructure clamp' driving and MEMS sensors for recording the associated strain/stress values. The nanomaterials of interest include carbon, boron nitride and B-C-N nanotubes, silicon, boron and aluminium nitride nanowires, BN nanoparticles, and MXene nanosheets. The values of Young's modulus, bending and tensile strengths, associated strains to fracture, and all peculiarities of deformations are unambiguously determined in real-time and under high spatial resolution (nm range) peculiar to the employed HRTEM technique.

*In situ* TEM Projects are supported through an Australian Research Council (ARC) Laureate fund FL160100089 (2017-2023). The author is grateful to coauthors at QUT, *i.e.,* Drs. J. Fernando, K. Firestein and C. Zhang, and NIMS, *i.e.,* Drs. D.M. Tang, O. Cretu, M.S. Wang, X.L. Wei, X. Zhou, M. Mitome, N. Kawamoto and Y. Bando, for their key contributions to *in situ* TEM projects over the years.

*Keywords: in situ TEM, nanomaterials, deformation, Young's modulus, tensile strength*

# Evaluation of Mechanical Properties of Irregularly Structured Nanomaterials - Utilization of Nanoindentation Techniques

**Dongyun Lee**

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## Abstract

Due to the functional uniqueness of nanostructures, there is increasing interest and research into their potential applications. Their mechanical behavior has also attracted significant attention. However, the synthesis of these nanostructures often results in a variety of shapes, many of which are irregular, posing challenges for mechanical observations. In this presentation, we aim to discuss the results of measuring and analyzing the mechanical properties of variously shaped nanostructures using nanoindentation techniques. By employing nanoindentation, we measured the mechanical characteristics within high-density samples of ZnO nanorods and $TiO_2$ nanotubes. We have proposed a method to determine the mechanical properties of individual entities in low-dimensional nanomaterial bundles using the Euler model and strain-energy density concept. Furthermore, we used nanoindentation to perform a qualitative comparison of the mechanical properties of ZnO nanosheets/ZnO nanorods and $Sb_2S_3/Cu_2S$ composites to phenomenologically understand material characteristics. We also intend to briefly mention various other applications of nanoindentation.

*Keywords: nanostructured materials, mechanical properties, nanoindentation*

# Research of Novel Graphene-Reinforced CuW Electrical Contacts for High Voltage Circuit Breaker

**Yi Ding[1]**, Zhen Pang[1], Tan Liu[1], Yu Han[1]

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**Abstract**

As the widely used electrical contact material of traditional high-voltage circuit breakers, copper-tungsten alloy has gradually reached a plateau in terms of conductivity, hardness and ablation resistance. It is difficult to support the requirements of contact materials for higher voltage and larger capacity circuit breakers in the development of power system. Graphene has attracted wide attention in recent years because of its good electrical conductivity, mechanical properties and high specific surface area. By enhancing the traditional copper-tungsten alloy material with graphene doping, it is expected to greatly improve the mechanical and electrical properties of traditional copper-tungsten alloy materials, and obtain novel graphene-reinforced CuW electrical contacts for high-voltage circuit breaker with excellent comprehensive properties. In this paper, graphene-reinforced CuW electrical contacts were prepared by vacuum infiltration. The microstructure of graphene-reinforced CuW electrical contacts and its influence on the mechanical, electrical propertie sand arc ablation resistance of electrical contacts were systematically studied by means of SEM, EDS, EBSD and other characterization methods. The strengthening mechanism of graphene-modified CuW electrical contacts is explained from the microscopic level.

*Keywords: Graphene; CuW Electrical Contacts; High-Voltage Circuit Breakers; Vacuum Infiltration; Strengthening Mechanism.*

# Exploring the Influences of Combined Pre-straining and Hydrogenation on the Nanomechanical Behavior of Selectively Laser Melted High-Entropy Alloy

**Zhe Gao[1]**, Dong-Hyun Lee[2], Yakai Zhao[3], A-Hyun Jeon[4], Pei Wang[5], Hyoung Seop Kim[6] Upadrasta Ramamurty[7], Jae-il Jang[8]

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**Abstract**

The combined effects of pre-straining and hydrogenation on the nanomechanical behavior of selectively laser melted (SLM) high-entropy alloy (HEA) samples are investigated. A series of nanoindentation experiments were performed on the samples that were pre-strained to different levels of strain and then electrochemically hydrogenated. To analyze the hydrogen behavior in a quantitative way, we performed TDS analysis and calculated the activation energy for hydrogen detrapping. The results are discussed in terms of the change in the main trapping sites for diffusible hydrogen before and after pre-straining.

*Keywords: Selective laser melting, high-entropy alloy, nanoindentation, hydrogenation.*

# Antiferromagnetic nanosheet $VS_xO_{2-x}$ for microwave absorption in high and low band by adjusting

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## Abstract

Developing broadband and high-efficiency electromagnetic wave absorbing material is an effective way to solve electromagnetic wave pollution. Usually single-phase materials cannot balance the magnetic permeability and dielectric properties. Herein, it is reported that VSxO2-x was successfully synthesized by a simple hydrothermal synthesis method, and its electromagnetic wave absorption properties were studied. The entry of oxygen modifies the structure of the sample to make the sample antiferromagnetic. When the reaction temperature reaches 170 °, the $VS_xO_{2-x}$ exhibits special electromagnetic wave absorption properties, and different thicknesses are dominated by different loss mechanisms. the reflection loss value of the sample at 13.45GHz can reach -11.45dB when the thickness is 3mm, and the reflection value can reach -12.13dB at 1.7GHz when the thickness is 5mm. It is worth noting that this special performance may be due to the well-matched impedance of the sample, the introduction of oxygen atoms, and the multiple reflections caused by its unique stacked structure. The significance of this study is to provide a new idea for the selection of the basic material of the electromagnetic wave absorber.

*Keywords: Electromagnetic wave absorption; Antiferromagnet; nanosheet*

# Technical **Oral Session _ Session 5**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 5 (N5)** **14:00 - 15:10, Nov. 21**

**Chair :** Teruyasu MIZOGUCHI (The University of Tokyo), Seonghwan Kim (Sejong University) **203, 2F**

14:00-14:30 **K-N1016** **[Keynote] Design of low-dimensional materials using artificial intelligence algorithm**
Jijun Zhao (Dalian University of Technology, China)

14:30-14:50 **I-N0397** **[Invited] Exploring Optimal Water Splitting Bifunctional Alloy Catalyst by Pareto Active Learning**
Yong Joo Kim (Kookmin University, Korea)

14:50-15:10 **I-N0952** **[Invited] Cloud Platform based on the Materials Genome Engineering Database Architecture for Data Storage and online Modelling**
Lei Zhang (University of Science and Technology Beijing, China)

# Design of low-dimensional materials using artificial intelligence algorithm

**Jijun Zhao**[1]

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## Abstract

Artificial intelligence refers to computer-imitating human cognitive abilities to learn and solve problems, and the related algorithms include genetic algorithms and machine learning, etc. Our research group has long been committed to developing a genetic algorithm CGA program that combines first-principles calculations. It has been successfully applied to search for ground state structures of over hundred kinds of atomic and molecular clusters, and has collaborated with experimentalists to discover a series of clusters with high stability and novel electronic properties. We have also carried out inverse design of PdS cluster photocatalysts using a modified CGA program. Recently, a deep learning based cluster graph attention network CGANet has been developed, which achieves efficient calculations for searching the ground state structure of silver clusters and predicting electronic properties. We have also developed a transition metal interconnection neural network for machine learning the magnetic anisotropy performance (MAE) of two-dimensional metal organic framework (MOF) materials.

**Keywords:** clusters, MOF, genetic algorithm, machine learning, graph attention network

# Exploring Optimal Water Splitting Bifunctional Alloy Catalyst by Pareto Active Learning

**YongJoo Kim[1]**

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## Abstract

Design of bifunctional multimetallic alloy catalysts, which are one of the most promising candidates for water splitting, is a significant issue for the efficient production of renewable energy. Owing to large dimensions of the components and composition of multimetallic alloys, as well as the trade-off behavior in terms of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) overpotentials for bifunctional catalysts, it is difficult to search for high-performance bifunctional catalysts with multimetallic alloys using conventional trial-and-error experiments. Here, an optimal bifunctional catalyst for water splitting is obtained by combining Pareto active learning and experiments, where 110 experimental data points out of 77946 possible points lead to effective model development. The as-obtained bifunctional catalysts for HER and OER exhibit high performance, which is revealed by model development using Pareto active learning; among the catalysts, an optimal catalyst ($Pt_{0.15}Pd_{0.30}Ru_{0.30}Cu_{0.25}$) exhibits a water splitting behavior of 1.56 V at a current density of 10 mA $cm^{-2}$. This study opens avenues for the efficient exploration of multimetallic alloys, which can be applied in multifunctional catalysts as well as in other applications.

*Keywords: entropy alloy, nanocatalyst, active learning, pareto learning, machine learning*

# Cloud Platform based on the Materials Genome Engineering Database Architecture for Data Storage and online Modelling

**Lei Zhang [1],** Xue Jiang [2], Jie He [3], Xiaotong Zhang [4], Yanjing Su [5]

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## Abstract

The construction of material data infrastructure has developed rapidly around the world, providing important support for data-driven materials discovery. With more and more application of the Materials Genome Engineering, the need for modern data infrastructures that facilitate the sharing of materials data and analysis tools is compelling in the materials community. An emerging architecture with high usability called Materials Genome Engineering Databases (MGED) was introduced to provide cloud-hosted services with features to simplify the process of collecting datasets from diverse data providers, unify data representation forms with user-centered presentation data model, and accelerate data discovery with advanced search capabilities. MGED also provides a standard service management framework to enable finding and sharing of tools for processing and analysing data. Based on MGED, the MaterHub platform has been established combined with cloud database, search engine, low-code workflow frameworks, as well as machine learning algorithm resource pools. It is an e-cooperation platform allowing data providers and users to design tasks and collaboratively build up machine learning models, schedule data, and obtain results online. At the same time, it can support model developers to deploy and deliver models for use by other scientists, facilitating the formation of a community for data-driven materials development and research. For example, an open-source web-based toolkit is provided and expected to serve as the basis for a general method to search for targeted materials using data extracted from the scientific literature.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: Materials Genome Engineering, Databases, Machine Learning, Workflow, Platform.*

# Technical **Oral Session _ Session 5**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 5 (O5)** **14:00 - 15:15, Nov. 21**

**Chair :** To be announced 401, 4F

14:00-14:30 **K-O0542** **[Keynote] Spent EV Battery Recycling for Securing Critical Raw Materials**
Jeong-Soo Sohn (Korea Institute of Geoscience and Mineral Resources, Korea)

14:30-14:45 **O-O0623** **Recovery of Lithium and Valuable Metals from the Waste Secondary Battery by Eco-friend Pyrometallurgical Process of Molten Carbonate Electrolysis**
Namhun Kwon (Korea Institution of Industrial Technology, Korea)

14:45-15:00 **O-O0745** **A Study of the Recovery Process of Lithium from Waste Lithium-Ion Battery (LIB) Black Powder Using Self-Propagating High-Temperature Synthesis (SHS) Process**
YONGKWAN LEE (Korea Institute of Industrial Technology, Korea)

15:00-15:15 **O-O0766** **Thermodynamics of MgO solubility in slag for pyrometallurgical treatment of spent LIB**
Se Hyeon Nam (Hanyang University, Korea)

# Spent EV Battery Recycling for Securing Critical Raw Materials

**Jeong-soo Sohn[1],** Hong-in Kim[1], Soo-kyung Kim[1], Dong-hyo Yang[1]

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**Abstract**

The use of eco-friendly vehicles was proposed as part of a plan to solve the global warming problems and practice carbon neutrality by 2050. Accordingly, the demand for battery raw materials used in eco-friendly vehicles is rapidly increasing, and much attention is being paid to securing critical raw materials to enhance the competitiveness of the domestic electric vehicle industry and the K-battery industry.

In particular, as one of the ways to secure key raw materials such as lithium, nickel, and cobalt used in electric vehicle batteries, recycling spent electric vehicle batteries is drawing attention. Currently, recycling companies such as Umicore, Sungeel Hitech, BRUNP, GEM, and Huayu Cobalt are recycling scraps from battery manufacturing companies and small spent batteries from wireless electronic wastes such as mobile phones. But in the case of spent electric vehicle batteries, better economical recycling process should be developed.

In this study, detailed processes necessary for the commercialization of an economical electric vehicle battery recycling process were examined. In particular, the next three strategies were emphasized in order to secure critical raw materials from electric vehicle battery recycling. 1) the ability to manufacture high-purity metal compounds from black mass leaching solutions and sell them to the battery cathode material manufacturing company must be secured, 2) precursors manufactured through the co-precipitation method without solvent extraction process must be utilized in real battery industry for detailed application, 3) the cathode material manufactured by the direct recycling process must be used in the commercialized battery for a specific purpose.

*Keywords: electric vehicle battery, recycling, critical raw materials, cobalt, lithium*

# Recovery of Lithium and Valuable Metals from the Waste Secondary Battery by Eco-friend Pyrometallurgical Process of Molten Carbonate Electrolysis

**Namhun Kwon**[1], Yongkwan Lee[2], Myungsuk Kim[3], Mihye Lee[4], JaeHong Shin[5] and Kyoung-Tae Park[6*].

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## Abstract

Current vehicles are being replaced with EVs (Electric Vehicles) that use electrical energy. Since secondary batteries that are used as the main power of electric vehicles, have a constant lifespan of 8 years, accordingly, many operating countries are constructing various plans and policies to handle this issue. Valuable rare metals such as nickel, cobalt, lithium, and manganese which all has limited resource, are contained in the wasted cathode material, and it could be used as a useful high-quality source by recycling process. Thus, it was conducted that the recovery of existing resources from waste cathode materials through the eco-friendly Molten Carbonate Electrolysis (MCE) process. Through the process, lithium, the main recovery target element could be recovered in the form of lithium carbonate while valuable metals such as nickel and manganese were separated and precipitated. Even though this process does not require any acidic or organic solvent, showed high recovery results with more environmentally friendly than the commercial hydrometallurgical recovery method while the process was also relatively simple. Various analysis was performed in X-ray diffraction, X-ray fluorescence, and FE-SEM to confirm the status of the characteristic in recovered lithium carbonate and other precipitated metallic powder. and the thermodynamical calculation was conducted using the HSC chemistry to optimize the process conditions such as the electrode materials, crucible materials, composition of molten carbonate, and process temperature. In addition, through electrochemical analysis such as chronoamperometry (CA) and cyclic-voltammetry (CV), the correlation between electrode reaction tendency and lithium compound recovery rate was identified.

*Keywords: Lithium Ion Battery; Materials; Recycling; Electrolysis; Electrochemical.*

# A Study of the Recovery Process of Lithium from Waste Lithium-Ion Battery (LIB) Black Powder Using Self-Propagating High-Temperature Synthesis (SHS) Process

**YongKwan Lee**[1], Namhun Kwon[2], HyunChul Kim[3], MiHye Lee[4], JaeHong Shin[5], KyoungTae Park[6*]

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## Abstract

Lithium-ion batteries are currently the most prominent technology in the electric vehicle and e-mobility market, which has been rapidly growing recently. Among the various secondary batteries available, lithium-ion batteries have the best performance and are gaining increasing demand as the world focuses on carbon neutrality and the $CO_2$ emissions associated with fossil fuel use, thus positioning them as an energy source for electric vehicles. As the demand for electric vehicles increases, the number of used electric vehicle batteries, making the recycling of these waste batteries a global concern. Therefore, this study explores a Pyrometallurgical recycling process to recover lithium from the black powder of waste lithium-ion batteries (LIBs). Firstly, an optimized heat treatment process was developed to remove carbon and organic impurities from the black powder. Subsequently, the heat-treated black powder was mixed with a reducing agent, Mg, and subjected to self-propagating high-temperature synthesis (SHS) to separate lithium from the black powder in the form of lithium oxide ($Li_2O$). Thermodynamic calculations using FactSage were performed to optimize the conditions of the self-propagating high-temperature synthesis, such as the amount of the reducing agent, process pressure, and temperature. Furthermore, the mechanism of the self-propagating high-temperature synthesis for lithium recovery from the black powder was elucidated.

*Keywords: Lithium-Ion Batteries, Black Powder, Self-Propagating High-Temperature Synthesis, lithium oxide, recycling*

# Thermodynamics of MgO solubility in slag for pyrometallurgical treatment of spent LIB

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## Abstract

The competition to secure resources is intensifying due to limited resources. A Lithium-ion battery (LIB) contains valuable metals such as Nickel (Ni) and Cobalt (Co), so the research for recovering valuable metals by recycling them is mainly in progress. In the pyrometallurgical recycling process, MgO dissolution behavior into the slag is directly related to the life of the refractory. Therefore, understanding the thermodynamics of MgO solubility in the slag is highly important. However, the gap between the thermodynamic calculation data and the experimental value is raised as an issue, and this problem is a task to be solved.

The goal of the current study is to check the difference between calculated and experimental values and to understand the thermodynamic behavior of MgO dissolution according to the composition of iron-silicate based slags. A commercial thermochemical computing software, FactSage$^{TM}$ (ver. 8.2) was used to design the $SiO_2$-$Fe_tO$-MgO-MnO-$Al_2O_3$-$Li_2O$ multicomponent slags. First of all, the iron-based alloy was prepared and a metal-slag equilibrium experiment was conducted using a high purity MgO crucible under the condition of $p(O_2) = 10^{-10}$ atm at 1550℃. The $Fe_tO/SiO_2$ ratio, MnO, $Li_2O$, and $Al_2O_3$ contents were chosen as experimental variables. The chemical compositions of metals and slags as well as refractory samples were characterized by ICP-OES, XRD, SEM-EDS, C/S and NOH analyzer.

*Keywords: Lithium-ion battery (LIB), Pyrometallurgical recycling, MgO solubility, Slag, Thermodynamics, Refractory*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 6

November 21

16:00-18:00

# Technical **Oral Session _ Session 6**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 6 (A6)** — **16:00 – 17:25, Nov. 21**

**Chair :** Motomichi Koyama (Tohoku University) — Halla Hall A, 3F

16:00-16:20 **I-A0865** **[Invited] Overcoming the strength-ductility trade-off in metastable dual-phase heterogeneous structures using variable temperature rolling and annealing**
Wei Xu (Northeastern University, China)

16:20-16:40 **I-A0694** **[Invited] Hydrogen trapping role of nano austenite transformed from metastable carbide in high strength steel**
Yuantao Xu (Shanghai Jiao tong University, China)

16:40-16:55 **O-A0333** **Variation of tensile elongation degradation with grain size in a hydrogen-charged metastable high Mn**
Mohammad Moallemi (Pohang University of Science and Technology, Korea)

16:55-17:10 **O-A0375** **Hydrogen embrittlement in additively manufactured ultra-high strength maraging steels: from mechanistic understanding to H-tolerant structure design**
Shiqi Zhang (Wuhan University of Science and Technology, China)

17:10-17:25 **O-A0736** **Immersion-type hydrogen charging on a high strength martensitic steel with Zn-coating**
Ju-Hyun Baek (Korea University, Korea)

# Overcoming the strength-ductility trade-off in metastable dual-phase heterogeneous structures using variable temperature rolling and annealing

**Wei Xu**[1,a], Jun Hu[1,b], Xuyang Li[1,c], Zheming Zhang[1,d], Lingyu Wang[1,e], Yizhuang Li[1,f]

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## Abstract

A novel variable temperature rolling (VTR) and annealing process was conducted on a metastable austenitic stainless steel. Strain softening occurred during tensile straining in both cold rolled and cryogenic rolled-annealed steels, leading to low uniform elongations of only 2-3%. In contrast, thanks to the metastable dual-phase heterogeneous lamellar structure achieved via the VTR process, a ultra-high strength of over 1 GPa was obtained, and strain hardening led to a remarkable increase of uniform elongation up to 10%. The high strength and ductility are attributed to the significant work-hardening derived from the superior heterogeneous deformation-induced hardening and sustained transformation-induced plasticity effect.

**Keywords:** austenitic stainless steel; variable temperature rolling; heterogeneous lamellar structure; HDI hardening; TRIP effect

# Hydrogen trapping role of nano austenite transformed from metastable carbide in high strength steel

**Yuantao Xu[1,2],** Wei Li[1,2], Xuejun Jin[1,2]

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## Abstract

Due to the unpredictability of hydrogen induced delayed fracture, it often leads to catastrophic accidents and huge economic losses. Hydrogen embrittlement has become a potential threat that restricts the widespread application of high strength-plasticity steel materials. A new precipitation-induced reverse phase transformation process was designed in 3.3Ni low-carbon medium-manganese steel. During the tempering (T) process, $Mn_{12}C$ carbides rich in Mn are precipitated (with a Mn content of up to 42 wt.%). In the process of partitioning (P), the Mn rich fcc $M_{12}C$ metastable carbides in the grain are transformed to form gradient Mn composition, dispersed distribution, and fine-sized reversed austenite. Due to the excellent hydrogen storage capacity of austenite, the dispersed nano austenite within ferrite grains serves as a strong hydrogen trap site, which can significantly reduce the hydrogen concentration at defect locations such as dislocations, grain boundaries, and phase boundaries, and inhibit hydrogen induced brittle fracture. Under tensile conditions after pre-charging with hydrogen (5.9 ppm H), increasing the proportion of nano austenite within ferrite grains can significantly suppress hydrogen-induced ductility loss.

*Keywords:* Medium-manganese steel, Hydrogen embrittlement, Phase transformation, $Mn_{12}C$ carbides, Nano austenite

# Variation of tensile elongation degradation with grain size in a hydrogen-charged metastable high Mn

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**Abstract**

High-Mn steels with an austenitic microstructure have a good combination of tensile strength and elongation thanks to the twinning-induced plasticity (TWIP) effect. The austenite phase in these materials depending on the stacking fault energy may undergo the martensitic transformation which affects the mechanical properties of the alloys. Recent studies have reported despite possessing superior elongation these alloys show a premature fracture exposing to hydrogen environments which is called hydrogen embrittlement. In the present research, the hydrogen embrittlement of a metastable high Mn with two different grain sizes has been studied. Hydrogen was introduced into fine-grained (FG) and coarse-grained (CG) specimens by electrochemical charging in a 3% NaCl aqueous solution containing 3 g/L of NH4SCN at a current density of 50 A/m2 for 48 h at 90 °C. A remarkable difference in ε-martensite fraction between CG and FG was observed after hydrogen charging repressing a drastic elongation loss in CG compared with FG alloy. The significant hydrogen embrittlement in CG alloy was attributed firstly to higher hydrogen concentration per grain boundary unit area and secondly to the more severe hydrogen cracking in CG than FG alloy because of explosive hydrogen-enhanced ε-martensite formation. Concerning the latter, a huge fraction of hydrogen-enhanced ε-martensite with limited slip systems inside the austenite grain of CG can interfere with the deformation accommodation and rotation of austenite grains during the tensile loading thereby facilitating grain boundary crack development.

*Keywords: High Mn Steel; Hydrogen embrittlement; Twin-induced plasticity; Strain-induced martensite*

| O-A0375 |

# Hydrogen embrittlement in additively manufactured ultra-high strength maraging steels: from mechanistic understanding to H-tolerant structure design

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## Abstract

The utilization of additive manufacturing technologies, such as laser-powder bed fusion (LPBF), in fabricating maraging steel has gained increasing attention in recent years. However, the strength–hydrogen embrittlement (HE) resistance trade-off is a critical issue that restricts the application of LPBF maraging steel in hydrogen-containing environments. In this work, advanced hydrogen trap characterization and high-resolution electron microscopy techniques have been utilized to probe the hydrogen trapping sites and reveal the mechanisms of hydrogen-assisted cracking in LPBF maraging steel. Furthermore, based on the computational simulation and novel heat treatment processes, a novel strategy for design of a multi-scale and multi-dimensional hydrogen trap network in LPBF maraging steel, which enable simultaneous enhancement of the strength and HE resistance is proposed. This work provides new insight into the design of HE resistance steels fabricated by additive manufacturing and motivates the industrial application of LPBF maraging steels.

*Keywords: Hydrogen embrittlement; Additively manufacturing; Maraging steel; Hydrogen traps.*

# Immersion-type hydrogen charging on a high strength martensitic steel with Zn-coating

**Ju-Hyun Baek[1,2]**, Sang Cheon Park[3], Dae Cheol Yang[2], Han-Jin Kim[3], Ki-Seok Nam[3], Jihong Yoo[3], Taejeong Kim[3], Seok Su Sohn[2], Jin-Yoo Suh[1]*

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## Abstract

Immersion-type hydrogen charging is one of the ways to put atomic hydrogen into a metallic specimen by simply dipping a specimen into an acidic solution. However, during the process, loss of surface layer is inevitable due to the dissolution of metallic ions into the solution. The method has not been applied to a steel plate with Zn coating layer due to the faster dissolution rate of Zn than Fe in a typical acid. However, considering the simplicity and convenience of the charging method and related hydrogen embrittlement testing such as 4-point bending of a steel plate under immersion condition, it would be useful to find a way to charge hydrogen into a metallic structure by immersion without losing too much of the coating layer for a given time duration, since it is likely that the existence of the coating layer could also influence the hydrogen embrittlement behavior. In that context, in this study, immersion hydrogen charging into a high strength martensitic steel was carried out with and without Zn coating layer by immersion into hydrochloric acid (HCl) and $NH_4SCN$ solutions. It turned out that the $NH_4SCN$ solution effectively charge hydrogen into the steel for both steels with and without Zn-coating layer. Also, Zn-coating layer remained after the charging process when $NH_4SCN$ solution was used while no coating layer in metallic form was found for the cases of HCl immersion. Thermal desorption spectroscopy (TDS) was utilized to measure the total amount of hydrogen before and after the charging and cross-sectional observation and electrochemical method were used to evaluate the remaining Zn coating layer after immersion for different time duration.

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*Keywords: Hydrogen embrittlement, Hydrogen charging, Electro-galvanized, Martensitic steels*

# Technical **Oral Session _ Session 6**

## **SSymposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 6 (B6)** **16:00 -17:50, Nov. 21**

**Chair :** Tomoya Nagira (National Institute for Materials Science) 301, 3F

16:00-16:20 **I-B0226** **[Invited] In situ observation of solidification behaviors of Fe-Mn-Si alloy during TIG welding**
Tomoya Nagira (National Institute for Materials Science, Japan)

16:20-16:35 **O-B0243** **Time-resolved and in-situ observation of solidification in Fe–22mass%Mn–0.7mass%C alloy using X-ray imaging techniques**
Taka Narumi (Kyoto University, Japan)

16:35-16:50 **O-B0508** **FEM estimiation of interfacial strength of dissimilar Al/Fe arc weld through fracture analysis by X-ray tomography**
Yutaka Sato (Tohoku University, Japan)

16:50-17:05 **O-B0351** **Coupled numerical-experimental approach to access interfacial temperature during aluminum-steel dissimilar arc welding**
Benjamin Leflon (INSA Lyon, France)

17:05-17:20 **O-B0417** **Effect of citric acid coating treatment of zinc insert sheet on the liquid-phase diffusion bonding strength of A5052 aluminum alloy**
HUY NGUYEN QUANG (Gunma University, Japan)

17:20-17:35 **O-B1011** **Investigation of dissimilar laser beam welding between VCoNi-medium entropy alloy and 17-4 PH stainless steel**
Hadis Esmaeilpoor (Hanbat National University, Korea)

17:35-17:50 **O-B0903** **Complex Vibration Assisted Ultrasonic Metal Welding Used for Manufacturing Cylindrical Cell Lithium-ion Batteries**
Mounarik Mondal (Dong-Eui University, Korea)

# In situ observation of solidification behaviors of Fe-Mn-Si alloy during TIG welding

**Tomoya Nagira**[1], Fumiyoshi Yoshinaka[2], Takahiro Sawaguchi[3], Takayuki Yamashita[4], Yasuhiro Aoki[5], Hidetoshi Fujii[6]

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## Abstract

Recently, Fe-15Mn-10Cr-8Ni-4Si alloy (FMS alloy) has been applied to seismic steel dampers due to its excellent plastic fatigue life. The alloy is weldable by changing the solidification mode from that in the austenite (A) mode to that in the ferrite-austenite (FA) mode. However, the solid-state transformation from the ferrite to the austenite occurred during the cooling. Therefore, the effect of the solidification mode on the solidification cracking susceptibility has not been understood from the observation of the solidified specimen consisting of fully austenite. In our previous study, the techniques for the in situ observation of solidification behaviors for the Al alloy and stainless steel during TIG welding were developed using synchrotron X-ray imaging and diffraction. In this study, the in situ observation of solidification behaviors of the FMS alloy at the weld bead was conducted to examine the microstructural evolution and the effect of solidification mode on the solidification cracking behaviors. The effect of welding speed on the microstructural evolution was also examined. In the A mode solidification, the solidification cracking initiated at the center of the weld bead where the columnar γ-Fe dendrites impinged in the nearly parallel direction to each other and linearly propagated toward the welding direction. On the other hand, the specimen solidifying in a FA mode showed the unique solidification where the equiaxed γ-Fe dendrite nucleated in front of the growing columnar δ-Fe dendrite. The many equiaxed γ-Fe dendrite suppressed the initiation of solidification cracking.

*Keywords: Welding, in situ observation, solidification behavior, solidification cracking.*

# Time-resolved and in-situ observation of solidification in Fe–22mass%Mn–0.7mass%C alloy using X-ray imaging techniques

**Taka Narumi**[1], Kengo Fujita[2], Makoto Ohta[3], Ryoji Katsube[4], Hideyuki Yasuda[5]

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## Abstract

We performed time-resolved and in-situ observations using X-ray imaging techniques at SPring-8 (synchrotron radiation facility in Hyogo, Japan) to explore the primary phase selection in Fe–22mass%Mn–0.7mass%C alloy in which the primary phase is austenite phase (fcc structure, γ phase) in the equilibrium phase diagram. X-ray radiography shows that ferrite phase (bcc structure, δ phase), which is a metastable phase, nucleated as the primary phase during cooling from the melt. The growth velocity of the δ phase was 100–200 μm/s. As dendritic growth of the δ phase proceeded, the δ phase massively transformed into the γ phase as a solid state. When the δ-γ transformation reached the δ/L interface, growth of the γ phase was initiated in the remaining liquid phase. Because the undercooling against the γ phase was relatively high, the growth velocity of the γ phase was beyond several mm/s. The primary phase selection was elucidated at undercooling from 10 K to 100 K using time-resolved X-ray diffraction measurement. The δ phase nucleated at the various undercooling; thus, the primary phase selection was independent of undercooling. Overall, this study demonstrates that the solidification path of L → L + δ → L + γ → γ is selected in Fe–22mass%Mn–0.7mass%C alloy, which differs from the equilibrium phase diagram (L → L + γ → γ).

*Keywords: Solidification, Phase transformation, Advanced high strength steel (AHSS), X-ray radiography, time-resolved X-ray diffraction*

# FEM Estimation of Interfacial Strength of Dissimilar Al/Fe Arc Weld through Fracture Analysis by X-ray Tomography

Kiyoaki T. Suzuki[1], **Yutaka S. Sato[2]**, Shun Tokita[3], Jérôme Adrien[4], Sylvain Dancette[5]

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## Abstract

Dissimilar welding of aluminum to steel has been a long-running scientific and technological problem mainly for the automotive industry. It would allow to achieve new designs of optimized vehicle structures combining strength, lightweight and energy absorption ability. However, the weld strength is limited because brittle intermetallic compound (IMC) layers are inevitably formed at the weld interface. In a previous study, the authors' group clarified that addition of Ni to the weld interface improved the weld strength drastically. However, its impact on the crack propagation resistance of the IMC layer itself has not been examined yet. In this work, effect of Ni addition on the mechanical behavior of the Al/Fe welds was investigated by means of microstructure analysis, *in situ* mechanical tests under X-ray tomography and finite element (FE) analysis. *In situ* mechanical tests showed that the AlNi/Fe weld exhibited faster crack propagation at higher fracture load than the Al/Fe one. The interfacial crack propagation behavior imaged by tomography was fitted using inverse FE simulation with a cohesive zone model. From a wide range of tentative cohesive strength and toughness for the IMC layer, this study clarified that the interfacial strength of AlNi/Fe weld was about twice that of Al/Fe one without Ni addition.

*Keywords: Dissimilar welding, Al/Fe weld, X-ray tomograph, finite element modelling, intermetallic compounds*

# Coupled numerical-experimental approach to access interfacial temperature during aluminum-steel dissimilar arc welding

**Benjamin Leflon**[1], Sylvain Dancette[2], Thibaut Chaise[3], Christophe Le Bourlot[4], Nicolas Mary[5], Yujin Aoyama[6], Kiyoaki T. Suzuki[7], Yutaka S. Sato[8]

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## Abstract

Intermetallic compounds (IMC) developing at the faying surface during heterogeneous welding of aluminum to steel are known to limit the strength of the dissimilar joints. Their formation, thickness and microstructure are highly dependent on the local thermal cycle experienced during the welding process. The latter is difficult to measure experimentally and is itself highly sensitive to the welding conditions. Based on a few reference measurements of temperature *operando* during the TIG arc welding process, a coupled numerical-experimental procedure is presented in this work to assess the evolving 3D temperature field in the welds during the process. Once calibrated, the finite element model allows (i) to determine keypoints in the welded structure for the effective measurement of thermal gradients and (ii) to highlight the sensitivity of such keypoints to the welding conditions, in terms of welding parameters but also of boundary conditions. Using the model, the virtual space of welding conditions is explored afterwards with the aim of influencing the development of the IMC layer at the faying surface through the attainment of targeted thermal histories.

*Keywords: Aluminum-steel welds, TIG welding, temperature measurement, finite element modeling, intermetallic compounds.*

# Liquid-phase diffusion bonding of A5052 aluminum alloy using Zn insert sheets with zinc citrate coating

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## Abstract

This study proposes a diffusion bonding method using a metal insert between two aluminum alloy plates. The formation of oxide films on joint surfaces has been paid attention since the failure to remove these films prior to joining can result in reduced joint strength and failure to meet welding specifications.

A zinc sheet was inserted at the junction interface to form a liquid phase near the junction surface and remove the natural oxide film on the aluminum surface. The results show that the bond strength was highest when the Zn sheet was treated with citric acid for 4 minutes, and the unloading temperature was 83°C, achieving a maximum bond strength of 121 MPa. The effect of welding pressure on tensile strength was also studied, and the optimal welding pressure to achieve tensile strength without deforming the test piece was found to be 6 MPa. The microstructure of the weld was observed using a scanning electron microscope and correlated with mechanical properties.

Overall, this study demonstrates the potential of using zinc inserts for enhancing the strength of aluminum alloy joints through liquid-phase diffusion bonding and provides insights into the optimal parameters for achieving strong joints.

*Key Words*: Metal Salt Coating Treatment, Citric Acid, Liquid-Phase Diffusion Bonding, Aluminum Alloy, Bond Strength

# Investigation of dissimilar laser beam welding between VCoNi-medium entropy alloy and 17-4 PH stainless steel

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## Abstract

High or medium-entropy alloys (HEAs or MEAs) have garnered attention due to their promising mechanical responses and functional properties. These alloys are distinguished by formation of disordered single-phase solid solutions, with FCC, BCC, or HCP crystal structures, rather than intermetallic or multiphase alloys. Recently, MEAs emerging as a promising class of materials for various industrial applications such as nuclear, since their low-activation components and fewer elements give design and preparation advantages. In this respect, an equiatomic VCoNi-MEA with a single FCC phase was developed, which exhibited superior tensile properties of 1 GPa yield strength. In addition, functionally graded materials play a vital role in nuclear applications, tackling challenges like thermal stress management and temperature gradient control, enhancing performance, mechanical properties, and etc. To ensure cost-effectiveness, combining MEAs with cost-efficient materials like stainless steel in weld construction offers a balanced approach to maintain quality while managing costs. Considering the notable properties and weldability, 17-4 PH SS emerges as an ideal candidate for joining with MEA in nuclear applications. Laser beam welding is preferred for achieving strong and reliable weld joints between VCoNi-MEA and 17-4 PH SS, offering precise heat control, high energy density, narrow fusion zone, and reduced heat-affected zone. Microstructure characterization utilizing FE-SEM, EBSD and micro-XRD revealed exceptional bead quality, homogeneous elemental mixing, and absence of microsegregation or cracks. Mechanical properties exhibited outstanding strength of 850 MPa, ductility of 8.3%, and hardness comparable to the parent metals. Post weld heat treatment at 900°C further improved the mechanical characteristics.

***Keywords***: *medium entropy alloys; precipitation hardening stainless steel; dissimilar laser beam welding; post weld heat treatment*

# Complex Vibration Assisted Ultrasonic Metal Welding Used for Manufacturing Cylindrical Cell Lithium-ion Batteries

**Mounarik Mondal**[1], Seong-Beom Park[1], Ji Young Shin[1], Soomin Lee[1]
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In recent years manufacturing of electric vehicles (EVs) has been scaled up significantly to control harmful environmental emissions as most of the transportation industry contributes 25-30% of the annual $CO_2$ emission. Most EVs use lithium Ion Battery (LIB) and are mostly of three types: cylindrical, prismatic, and pouch. Among these, cylindrical shape batteries can withstand high temperatures and pressure without much deformation and provide better economy due to their well-versed production process. In manufacturing these types of batteries, the joining of Al/Al and Cu/Cu combinations in dissimilar thickness combinations is extensively used. Hence, in recent times a lot of research is being carried out to achieve a sound technique for joining these materials. Ultrasonic Metal Welding is a solid-state joining process for which it is mostly desired to be used as a joining method for non-ferrous alloys. Hence in this work, a novel circular trajectory-based complex vibration-assisted ultrasonic welding has been carried out to weld a 0.2 mm thick AA 1050 sheet with a 3 mm thick 3003 Al tab. The welds were carried out in both position and pressure control modes. An in-detailed correlation was studied between the weld input parameters (amplitude, weld time, pressure) and weld quality (such as weld size, bond depth, bond density, dynamic recrystallization, and joint strength). It was found that the combination of both the vibrational amplitude and pressure influenced the dynamic recrystallization inside the weld, which further influenced the final quality of the weld.

**Keywords:** Cylindrical Cell Battery welding, Ultrasonic Welding, Complex Vibration, Dynamic Recrystallization

# Technical **Oral Session _ Session 6**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 6 (C6)** **16:00 - 17:35, Nov. 21**

**Chair :** Xiping GUO (Northwestern Polytechnical University), Kyosuke Yoshimi (Tohoku University) 201A, 2F

16:00-16:30 **K-E1139** **[Keynote] Mechanical behavior of titanium lattice structures fabricated by powder bed fusion**
Laichang Zhang (Edith Cowan University, Australia)

16:30-16:50 **I-C0291** **[Invited] Variations in the positive temperature dependence of yield stress for Co3(Al, W)–Co3Ti pseudo-binary intermetallic compounds**
Katsushi Tanaka (Kobe University, Japan)

16:50-17:05 **O-C0509** **Study on the effect of infinitesimal potassium doping on the ductile-to-brittle transition temperature of tungsten as a plasma-facing material**
Jeongseok Kim (Seoul National University, Korea)

17:05-17:20 **O-C0447** **For the oxidation-resistant MoSiB-based ultrahigh-temperature materials**
Mi Zhao (Huazhong University of Science and Technology, China)

17:20-17:35 **O-C0227** **Effect of Nb on Phase Equilibria and Mechanical Properties of Mo-Ti-C Alloys**
Xinyu Yan (Tohoku University, Japan)

# Mechanical behavior of titanium lattice structures fabricated by powder bed fusion

**Lai-Chang Zhang**[1]

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## Abstract

Lattice structures (Periodic cellular materials) are a type of architectures constructed by an array of spatial periodic unit cells with edges and faces. Although lattice structures exhibit a range of superior properties, such as low elastic modulus, high specific stiffness and strength, large surface area, a large number of internal pores, and relatively low-stress level, the manufacturing by traditional technologies and the optimization of properties of lattice structured are limited because of poor control over the morphological characteristics of the pore network. The recent advances in metal additive manufacturing (AM) technologies have enlarged the design and manufacturing possibilities for lattice structures, which provides lattice structures with promising solutions for a variety of applications. This work presents the recent progress of additive manufacturing and enhanced mechanical and catalytic performance of lattice structures. The selective laser melting (SLM) produced and electron beam melting (EBM)-produced beta-type biomedical titanium lattice structures, as potential load-bearing implants, demonstrate excellent mechanical properties in terms of high super-elasticity, low Young's modulus and high compression strength, high energy absorption and fatigue properties.

*Keywords: Additive manufacturing; Titanium; Lattice structure; Mechanical behavior; Fatigue*

# Variations in the positive temperature dependence of yield stress for $Co_3(Al, W)$–$Co_3Ti$ pseudo-binary intermetallic compounds

**Katsushi Tanaka**[1], Takeshi Teramoto[2]

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## Abstract

Composition dependence of positive temperature dependence of yield stress for $Co_3(Al, W)$–$Co_3Ti$ pseudo-binary alloy with the $L1_2$ structure have been investigated. The temperature dependence of the yield stress of polycrystalline specimens have been determined from 293 to 1273 K. The onset temperatures for the positive temperature dependence of yield stress for pseudo-binary compounds are located between that of $Co_3(Al, W)$ and $Co_3Ti$. The composition dependence of the positive temperature dependence of yield stress is estimated from the physical properties of $Co_3(Al, W)$ and $Co_3Ti$. The estimated parameters for describing the positive temperature dependence of yield stress almost represent the experimental results, indicating that the positive temperature dependence of yield stress for pseudo-binary compounds can be predicted from the physical properties of the base compounds.

*Keywords: Positive temperature dependence of yield stress, $L1_2$ compound, Composition dependence, Stacking fault energy, Activation energy*

# Study on the effect of infinitesimal potassium doping on the ductile-to-brittle transition temperature of tungsten as a plasma-facing material

**Jeongseok Kim[1],** Guensik Min[2], Sungmin Lee[3], Yeonju Oh[4], Simoon Sung[5], Hwangsun Kim[6], Hyoung Chan Kim[7], Ill Ryu[8,*] and Heung Nam Han[9,**]

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## Abstract

Tungsten is the most promising candidate as a plasma-facing material due to its unique properties, including a high melting point (3422°C), low sputtering yield, and excellent thermal conductivity. Nevertheless, the high ductile-to-brittle transition temperature (DBTT) of tungsten strongly limits its operational window. Previous studies have indicated that potassium doping can lower the DBTT of tungsten, thereby overcoming its inherent brittleness. However, the underlying mechanism of this phenomenon is still unknown. Therefore, this study aims to investigate the mechanism of reducing the DBTT of tungsten by potassium doping through experiments and simulations. Potassium-doped tungsten (K-doped W) was fabricated using the spark plasma sintering method. TEM-EDS analysis revealed the formation of nano-sized potassium bubbles through vaporization. For comparison, annealed pure tungsten was prepared

by fully annealing high-purity tungsten above the recrystallization temperature. XRD peak analysis showed that the dislocation densities of K-doped W and annealed pure tungsten were comparable. Uniaxial tensile tests confirmed that the DBTT of K-doped W was reduced, and the tensile toughness of K-doped W was improved compared to annealed pure tungsten. Furthermore, nanoindentation tests were conducted to characterize the microscopic mechanical properties of tungsten. The results indicated that the maximum shear stress for yielding of K-doped W was lower than that of annealed pure tungsten. Molecular dynamics and dislocation dynamics simulations elucidated that the nano-sized bubble induces stress concentration in localized areas near the bubble, thus facilitating the nucleation of dislocations in tungsten. Consequently, it decreases the macroscopic stress for yielding and contributes to the reduction in DBTT.

*Keywords: Tungsten; Potassium bubble; Ductile-to-brittle transition temperature; Nanoindentation; dislocation dynamics simulation;*

# For the oxidation-resistant MoSiB-based ultrahigh-temperature materials

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## Abstract

Ultrahigh-temperature structural materials beyond Ni-based superalloys contribute to high-temperature technologies in the fields such as aerospace engineering and land-based power plants. For example, MoSiB alloys are kinds of promising candidates for ultrahigh temperature application, where high-efficiency engines might benefit from their high melting points, good phase stability and good creep resistance. However, the balance between room-temperature fracture toughness and high-temperature oxidation resistance is hardly achieved for them since high volume fraction of solid-solution phase (BCC-$Mo_{ss}$) and high Si content are impossible to simultaneously obtain according to the ternary phase diagram. Recently, a $Ti_5Si_3$-containing MoSiB-based alloy had been developed through macro-alloying of Ti to the ternary system. In the quarternary alloys, it is not difficult to preserve both high volume fraction of $Mo_{ss}$ and high Si content at the same time because Ti is a typical BCC-stabilized alloying element. However, the high-temperature oxidation resistance of this newly developed MoTiSiB alloy is still far from satisfactory and its oxidation mechanism has not been totally revealed. In this study, we tell the history from MoSiB to MoTiSiB alloys. The phase equilibrium and microstructure were analyzed. Especially, high-temperature oxidation behavior was investigated. Oxidation kinetics, oxidation products and oxidation mechanism were discussed. This can promote the design and development of novel ultrahigh-temperature materials.

*Keywords: MoSiB alloys; alloy design; microstructure; high-temperature oxidation.*

# Effect of Nb on Phase Equilibria and Mechanical Properties of Mo-Ti-C Alloys

**Xinyu Yan[1]**, Junfeng Du[2], Hiromu Matsuura[3], Xi Nan[4], Shuntaro Ida[5], Kyosuke Yoshimi[6]

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## Abstract

Mo-Ti-C eutectic composites are promising as high-temperature structural materials because of their high strength at high temperatures and fracture toughness at room temperature. Mechanical properties must be further improved to facilitate aerospace and power generation applications. The Nb addition offers a promising solution to optimize the microstructure further and improve the mechanical properties. Therefore, this research aims to investigate the effects of Nb addition on Mo-Ti-C alloys.

Several Mo-Ti-C and Mo-Nb-Ti-C alloys were prepared in an Ar atmosphere and then annealed at 1500 °C for 100 hours. Scanning electron microscopy (SEM) and electron probe microanalysis (EPMA) were used to determine the liquidus surface projection and isothermal section at 1500 °C of the (Mo,Nb)-Ti-C pseudo-ternary system. Microstructural characterization reveals that Nb addition stabilizes TiC phase and suppresses the formation of $Mo_2C$ phase. The mechanical properties of the alloy were evaluated by microhardness and four-point bending tests at room temperature. Nb addition decreased the hardness of Mo-Ti-C alloys. The fracture surface observations revealed that both Mo solid solution ($Mo_{ss}$) and TiC acted as toughness-enhancing phases in the Nb-added 50Ti10C alloy. Then the fracture toughness value approached 16 $MPa(m)^{1/2}$.

*Keywords: Multiphase alloys, Microstructure, Phase equilibria, Fracture toughness*

# Technical **Oral Session _ Session 6**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 6 (D6)** **16:00 -17:55, Nov. 21**

**Chair :** Young Min Kim, Korea Institute of Materials Science, Eiji Abe, University of Tokyo Samda Hall A, 3F

16:00-16:30 **O-D0128** **[Keynote] Recent evolutions and new applications of SEN Mg alloys**
Bong Sun You (Korea Institute of Materials Science, Korea)

16:30-17:00 **K-D1105** **[Keynote] Development of Rare-earth Free High Strength Magnesium Alloys**
Yuansheng Yang (Chinese Academy of Sciences, China)

17:00-17:20 **I-D0322** **[Invited] Magnesium Alloy Sheet for Front Hood Project in Japan**
Kazumasa Yamazaki (Nippon Kinzoku Co.,Ltd., Japan)

17:20-17:40 **I-D1142** **[Invited] Research and development of Ti particle reinforced Mg composites with enhanced strength and ductility**
Xianhua Chen (Chongqing University, China)

17:40-17:55 **O-D0927** **Effect of addition of Ca in liquid Mg on the formation of Mg/Ti composites fabricated by liquid metal dealloying**
Jee Eun Jang (Kyungpook National University, Korea)

# Recent evolutions and new applications of SEN Mg alloys

**Bong Sun You**[1], Hongxiu Liu[2], Wen Ding[3], Jun Ho Bae[4], Young Min Kim[5]

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## Abstract

The main reason for abandoning magnesium alloy after the beginning of the active use in the automobile and aircraft industries in the 1940s, which is still the key issue not to use very large amounts of magnesium alloys in the automobile industry, is its high corrosion rate compared with other metals.

KIMS have been studied on new corrosion resistant magnesium alloys by the addition Ca and Y together. A controlled amount Ca and Y containing phases and the formation of multi-layered protective oxides consisting of CaO, Y2O3, MgAl2O4, and MgO effectively improve the corrosion resistance. This paper introduces the mechanism of corrosion resistance of Ca and Y containing alloys, and compares the corrosion behaviour with that of commercial alloys. Also, it introduces field test results on several items which are made by die casting, billet making and extrusion processes for the application in electronic, automotive and aerospace industries.

*Keywords: Mg alloy, High Al content, Cooling rate, Corrosion behaviour.*

# Development of Rare-earth Free High Strength Magnesium Alloys

**Yuansheng Yang[1],** Tianjiao Luo[2], Qiuyan Huang[3], Ce Zheng[4], Yingju Li[5], Xiaohui Feng[6]

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## Abstract

As the lightest metal structural material, magnesium alloy has broad application prospects in light weight and energy saving, and plays an important role in the fields of transportation, aerospace, electronic communication and so on. Nowadays the application of magnesium alloy is from non-load-bearing parts to load-bearing structural parts, so it needs higher strength and toughness coordination to achieve good service performance. It is also necessary to meet the requirements of efficient preparation and low cost considering the industrial scale application. In our study, rare-earth free magnesium alloys with high Strength are developed by multi-alloying and nano-phase precipitation strengthening. Based on the thermodynamic phase diagram calculation and the first-principles calculation, the kinds of main elements and the main types of nano-precipitated phases as well as the precipitation range of the strengthened phase in the alloy are determined, and the micro-alloying elements that promote the precipitation of the nano-strengthened phase are determined. The morphology, quantity, and orientation of the nano-precipitated phase are controlled by multistage-aging processing. The comprehensive mechanical properties of the rare-earth free magnesium alloys are greatly improved through co-regulation of nano-precipitation strengthening and grain boundary strengthening. The developed rare-earth free cast magnesium alloys and wrought magnesium alloys have been applied successfully in transportation vehicles and other fields.

*Keywords: Magnesium alloy; precipitation strengthening; nano-precipitated phase; rare-earth free; micro-alloying.*

# Magnesium Alloy Sheet for Front Hood Project in Japan

**Kazumasa Yamazaki**[1], Yasumasa Chino[2], Masahiko Satou[3], Xinsheng Huang[4], Isao Nakatsugawa[4], Takumi Kozaki[5], Miho Haruki[5], Masahiro Umeda[5], Ryohei Takayama[6], Kenichi Nakamura[6]

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## Abstract

The NEDO-commissioned "Development of Innovative New Structural Materials and Other Technologies" conducted a project to reduce the weight of automobiles. This project studies to application of Magnesium rolled sheets to automobile bodies. Applying Magnesium sheets to panels is expected to be more effective in weight reduction than structural members. Therefore, we proceeded with the project to produce a prototype front hood with a similar shape using an actual car model with Aluminum exterior panels. Other goals included lowering the stamping temperature from approximately 250°C to 150°C, developing a simultaneous conversion treatment method for Magnesium, Aluminum, and galvanized steel in consideration of the coating process on the actual production line, and preventing galvanic corrosion when joining dissimilar metals. We used the Magnesium sheets joined by FSW. Model forming was conducted in advance to confirm the forming conditions. As a result, although the plate thickness was 1.2 times that of Aluminum, we achieved the desired goals in terms of panel rigidity, pedestrian protection performance, and corrosion resistance. And we achieved an 18% weight reduction compared to the Aluminum front hood.

The topic area : D JIM

*Keywords: Rolled Magnesium Sheet, Weight reduction of AUTO Body, Front-Hood, Simultanious Conversion Chemical Treatment, Pedestrian Protection*

# Research and development of Ti particle reinforced Mg composites with enhanced strength and ductility

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Conventional magnesium (Mg) based composites are often difficult to achieve the trade-off between strength and ductility due to the occurrence of brittle ceramic particles. The titanium (Ti) metal particles, which show better wettability and ductility than ceramic particles, are potential reinforcements to simultaneously enhance the strength and plasticity of Mg alloys. However, the distribution of Ti particles and the interfacial bonding strength are the critical challenges for the Ti reinforced Mg composites. This presentation placed emphasis on the optimization of Ti particle distribution and the tailoring of interface microstructures to develop Mg composites with high strength and plasticity. Firstly, different fabrication techniques, casting parameters and Ti particle types (shape, size, compositions, etc.) were designed to achieve a relatively homogeneous dispersion of reinforcements and the improved mechanical properties. Secondly, the interfacial microstructures are systematically tailored and optimized by distinct manufacturing methods in Ti reinforced composites. The lattice parameters, structures, elemental segregation and crystallographic orientation relationship at Ti/Mg interface were clearly revealed using HRTEM. The relationship between interface microstructures and the mechanical properties was compared and discussed. In conclusion, the research trends and future design of Ti reinforced Mg composites are proposed to develop Mg alloys with both high strength and ductility.

*Keywords: Magnesium, Titanium, Composites, mechanical properties, ductility*

# Effect of Ca addition in the liquid Mg on morphological evolution and mechanical properties of Mg/Ti composite fabricated by liquid metal dealloying

**Jee Eun Jang[1]**, Seung Ho Lee[2], Soo-Hyun Joo[3], Sung Hyuk Park[4,*]

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## Abstract

The liquid metal dealloying (LMD) has recently developed as a novel technique to fabricate bi-continuous composite structures by utilizing miscibility of alloying elements. The LMD is easily conducted by immersing the precursor in the liquid metal in certain time. When the precursor is immersed in a liquid metal, alloying elements in the precursor that are highly miscible with the liquid metal are dissolved into the melt, correspondingly, the composite can be fabricated after the melts fill the empty space. Mg/Ti composite is promising as a biocomposite material due to the similar elastic modulus to bone and high biocompatibility. The LMD process is expected to enable the fabrication of Mg/Ti composite with a three-dimensional connected nanostructure, exhibiting enhanced properties. Previous LMD studies have investigated on the effect of process conditions such as precursor composition and melt temperature to improve the properties of composite. Since the miscibility differences between alloying elements are determinant driving forces for the LMD process, miscibility tuning by adding alloying elements is expected to improve the properties of LMDed composite. In this study, the effect of Ca addition in liquid metal on the LMD process to fabricate the Mg/Ti composite was investigated. Mg/Ti composite was fabricated by utilizing a Mg-*x*Ca liquid metal containing 1 to 10 wt.% Ca addition, which has excellent biocompatibility to nervous system. The LMD reaction behavior corresponding to dealloying kinetics and morphological evolution, and mechanical properties of the composites with variant Ca content were characterized by comparing the microstructure analysis and hardness value.

***Keywords***: *Liquid metal dealloying, Mg/Ti composite, 3D bicontinuous structure, Biomaterials, Miscibility*

*This work was supported by the National Research Council of Science & Technology (NST) grant by the Korea government (MSIT) (CRC23011-000)*

# Technical **Oral Session _ Session 6**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 6 (E6)** **16:00 -17:40, Nov. 21**

Chair : Andrew Ang (Swinburne University of Technology), Yoon Suk Choi (Pusan National University) Halla Hall B, 3F

16:00-16:20 **I-E0496** **[Invited] Thermal stability of non-equilibrium microstructural features of additively manufactured austenitic stainless steel**
Cecilie Funch (The University of Sydney, Australia)

16:20-16:40 **I-E0307** **[Invited] Crystallographic texture control via metal additive manufacturing**
Takayoshi NAKANO (Osaka University, Japan)

16:40-16:55 **O-E0266** **Controlling microstructure of additive-manufactured Al-Fe-Cu alloy for high strength and thermal conductivity**
Yue Cheng (Nagoya University, Japan)

16:55-17:10 **O-E0469** **On the microstructure evolution in Inconel 718 alloy fabricated by laser powder-bed fusion**
Shuai Wang (Southern University of Science And Technology, China)

17:10-17:25 **O-E0182** **Nano-scaled microstructure characterization and analysis of 316L stainless steel fabricated by laser powder bed fusion**
FEI SUN (Nagoya University, Japan)

17:25-17:40 **O-E0443** **Materials and process innovations in laser-directed energy deposition high-strength aluminium alloys**
Chaolin Tan (Agency for Science, Technology And Research (A*STAR), Singapore)

# Thermal stability of non-equilibrium microstructural features of additively manufactured austenitic stainless steel

**Cecilie V. Funch**[1,2], Flemming B. Grumsen[3], Thomas L. Christiansen[4], Marcel A.J. Somers[5]

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## Abstract

The rapid cooling rates and cyclic thermal history of the laser powder bed fusion additive manufacturing process are known to produce unconventional or non-equilibrium microstructures in otherwise common conventional alloys. One of the most widely adopted materials for metal additive manufacturing is the austenitic stainless steel alloy AISI 316L. When this austenitic stainless steel is produced by laser powder bed fusion the microstructure is generally characterized by primary austenite grains elongated in the direction of the largest heat flux. Inside the primary grains, columnar cells are collected in domains of cells with a similar crystallographic orientation and a small misorientation to neighbouring domains. The cell walls are enriched in the ferrite-stabilizing elements Cr and Mo and contain dense dislocation tangles. The walls are decorated with small amorphous spherical silicates. This study investigates how these microstructural features evolve during thermal exposure in the temperature range of 400-1100 °C. The cell structure is found to be thermally stable up to about 800 °C with a gradual decrease of dislocation density, while the domain boundaries remain stable and present as fine low-angle grain boundaries. The evolution of the amorphous silicates is investigated in detail using carbon extraction replicas. At intermediate temperatures (700-800 °C), σ-phase precipitates adjacent to the silicates, while at high temperatures (1000-1100 °C) the silicates are replaced by larger oblong Cr,Mn-based oxides.

**Keywords:** Additive manufacturing, stainless steel, microstructure evolution, heat treatment.

# Crystallographic texture control via metal additive manufacturing

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## Abstract

The attractiveness of metal additive manufacturing (AM) lies not only in the creation of complex 3D shapes, but also in the ability to control mechanical properties and mechanical isotropy/anisotropy by controlling the crystallographic texture of metals. In this talk, I will present the latest findings on the control of crystallographic textures using mainly laser powder bed fusion (L-PBF), which our group has been making vigorous efforts in recent years. For example, in β-type titanium alloys, the laser conditions can vary wide range of textures from randomly oriented polycrystalline to single-crystal-like textures, and the scanning strategy can change the crystal orientation direction, and produce the corresponding isotropic/anisotropic Young's modulus. Furthermore, the induction of anisotropy in biological cells and tissues by fine shape control will be presented. The possibilities for metal AM are expanding.

This work was supported by CREST-Nanomechanics [grant number JPMJCR2194] from the Japan Science and Technology Agency.

***Keywords:*** *Crystallographic texture, Anisotropy, Powder bed fusion*

# Controlling microstructure of additive-manufactured Al-Fe-Cu alloy for high strength and thermal conductivity

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## Abstract

In the present study, the microstructure of Al–2.5Fe–2Cu (wt%) ternary alloy samples manufactured by laser powder bed fusion (L-PBF) process was systematically characterized, and its variation due to subsequent annealing at various temperatures ranging from 200 to 500 °C was investigated. Mechanical properties and thermal conductivity of the L-PBF manufactured and subsequently annealed specimens were measured. The as-manufactured sample exhibits a clear melt-pool structure containing numerous fine particles of the $Al_{23}CuFe_4$ phase homogeneously distributed inside melt pools. Nanoscale precipitates were homogenously formed inside the α-Al matrix after the annealing at 300°C, whereas relatively coarsened $Al_{13}Fe_4$ phases were often observed in the 500°C annealed sample. The as-manufactured specimen exhibited a high tensile strength of approximately 350 MPa and a relatively low thermal conductivity of approximately 140 $Wm^{-1}K^{-1}$. The 300 °C annealing increased the thermal conductivity to 180 $Wm^{-1}K^{-1}$ without a loss of strength (and ductility), whereas the annealing at a high temperature of 500 °C significantly reduced the tensile strength. The mechanism of managing both high strength and thermal conductivity will be discussed using the experimental results of microstructural characterizations for the as-manufactured and 300 °C annealed samples.

***Keywords:*** *additive manufacturing, Al-Fe-Cu alloy, tensile strength, thermal conductivity, microstructure*

# On the microstructure evolution in Inconel 718 alloy fabricated by laser powder-bed fusion

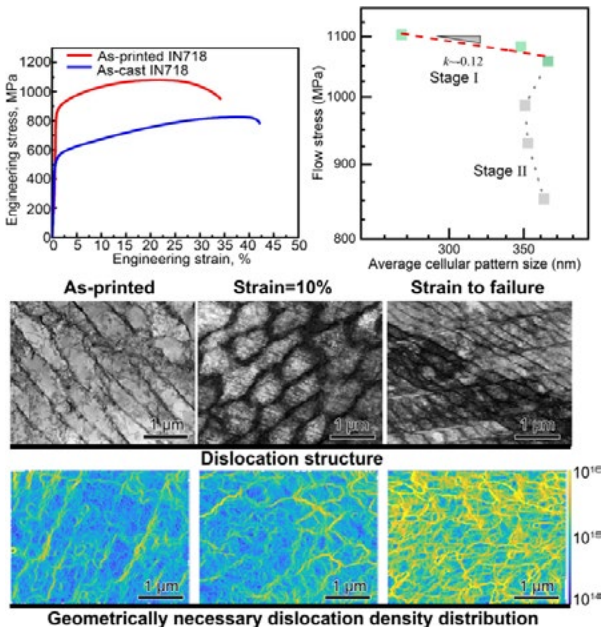
**Shuai Wang**[1], Minglin He[1]

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## Abstract

Many experimental observations have proved that the characteristic wavelength of dislocation pattern, e.g., a cell size, is inversely proportional to the flow stress, which is known as the empirical scaling law. In this work, we systematically studied the development of solidification-induced cellular patterns and dislocations in Inconel 718 alloy that was processed with laser powder-bed fusion technology. Although the appearance of the cellular pattern was almost the same as the deformation-induced dislocation structure, their microstructure development as a function of external stress was utterly different.

Our observation indicated that dislocation evolution is a two-stage process. At a tensile strain lower than 10%, the size of the cellular pattern was independent of flow stress. At higher strain levels, the cellular pattern size decreased; however, the maximum reduction obtained at the strain-to-failure was only ~27% of the undeformed cell size. During the stage of cell size reduction, the flow stress was approximately proportional to $\sim d_c^{-0.12}$ ($d_c$ is the average cell size). The high structural stability of the solidification-induced cellular pattern was attributed to the formation of secondary phases, solute segregation, vacancies, and pre-existing high-density dislocations at the cellular boundaries. The evolution of the solidification-induced cellular pattern cannot be described by Taylor-type ($\sim d_c^{-1}$) or Hall-Petch-like ($\sim d_c^{-0.5}$) relationships.




*Keywords: Laser powder-bed fusion; Inconel 718 alloy; Cellular pattern; Dislocation structure; Strengthening*

# Nano-scaled microstructure characterization and analysis of 316L stainless steel fabricated by laser powder bed fusion

**Fei Sun [1]**, Toshio Ogawa[2], Yoshitaka Adachi[1], Kazuhisa Sato[3], Goro Miyamoto[4,5], Takuya Ishimoto[6], Takayoshi Nakano[7,8], Yuichiro Koizumi[7,8]

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## Abstract

Metal additive manufacturing enables producing complex geometric structures with high accuracy and breaks the design constraints of traditional manufacturing methods. Laser powder bed fusion, a typical additive manufacturing process, presents a challenge in experimentally understanding the nano-scaled microstructure-process relationship regarding the wide range of process parameters. This study aims to reveal the novel nanoscale structural features in 316L stainless steel by laser powder bed fusion by advanced scanning transmission electron microscopy.

316L stainless steel was fabricated by laser powder bed fusion using a 3D printer (EOSM290, EOS GmbH, Germany) equipped with a Yb-fiber laser by the "X-scan strategy," i.e., the laser beam was scanned bidirectionally along the x-axis without rotation. A basic set of process parameters was selected for generating the studied specimen: laser power 250W, laser scan speed 1000mm/s, layer thickness 40 μm, and laser hatching distance 80 μm. All the microstructural analyses were performed in the as-built specimen without any heat treatment.

Here we show that the slender columnar grains were confined to the centreline of the melt pool along the build direction, and the columnar cell structure at the side branching of the melt pool grew along orthogonal directions to follow drastic changes in a thermal gradient across adjacent melt pools. Novel nano-scaled modulated structures have been observed in the dislocation cells parallel to the laser scan direction, which was mainly caused by the elastic strain involving the thermal gradient inside the melt pool and across adjacent melt pools as well as the effective strain field in the dislocation cell interiors. An in-depth understanding of microstructure developments is worthy of fabricating high-performance materials by controlling the additive manufacturing process.

*Keywords: laser powder bed fusion, 316L stainless steel, dislocation cell, modulated structure, transmission electron microscope*

# Materials and process innovations in laser-directed energy deposition high-strength aluminium alloys

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## Abstract

Additive manufacturing (AM) offers design freedom and manufacturing flexibility for processing high-performance complex components. High-strength aluminium (Al) alloys (e.g., AA5000 and AA7000 series alloys) are widely used in aerospace due to their high strength-to-density ratio and superior ductility; however, AM high-strength Al alloys are still challenging due to the intrinsic properties (e.g., low laser absorption and high cracking tendency). Although some success in processing high-strength Al alloys has been achieved so far with laser powder bed fusion (LPBF), these solutions have not yet been translated effectively to the laser-directed energy deposition (LDED) process due to evident differences in deposition environment and thermal histories. State-of-art of LDED Al alloys suggests a bottleneck in achieving yield strength higher than 350 MPa. Therefore, customized Al alloys materials for LDED for achieving high strength are highly demanded. This work will introduce materials and process innovations in LDED Al alloys to obtain high strength and high ductility. Several novel high-strength Al alloys customized for LDED will be introduced in terms of printability examination, microstructure evolution and mechanical properties. Innovative LDED processes, such as green laser deposition and coaxial wire deposition, are also investigated to understand the effect of process on the achievable mechanical properties. The synergic invocations in materials and processes achieved an excellent combination of strength-ductility in LDED Al alloys, superior to a wide range of Al alloys processed by LDED. This work highlights materials design for AM, rather than following conventional composition, to unlock the unparalleled potential of AM high-performance components.

***Keywords***: *Additive manufacturing; Laser printability; New materials, High-strength Al alloy; Particle reinforcement.*

**Presenting author**: **Dr Chalin Tan**, Scientist, Principal Investigator and Doctoral Supervisor at the A*STAR. He is a **Fellow** of International Association of Advanced Materials (IAAM) and ranked 2022 World's Top 2% Scientists published by Stanford University. He is on **Editorial Board** of flagship journal ***Int. J. Mach. Tools Manuf.*** (IF 10.33) and **Youth Editor** of ***Int. J. Extreme Manuf.*** (IF 10.03) and ***J. Mater. Sci. Technol.*** (IF 10.32). His research interests are additive manufacturing, 4D printing, heterostructural materials, and multi-scale structure-property characterizations.

# Technical **Oral Session _ Session 6**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 6 (F6)** **16:00 - 17:30, Nov. 21**

**Chair :** Hyunjung Shin (Sungkyunkwan University), Qing Wang (Dalian University of Technology) 202A, 2F

16:00-16:30 **K-F0548** **[Keynote] Characterization of a Cobalt-Chromium-Molybdenum Alloy Subjected to Surface Mechanical Attrition Treatment**
Gwénaëlle Proust (The University of Sydney, Australia)

16:30-16:50 **I-F0159** **[Invited] Formation of Porous Ni-Pt Alloy using the Molten Salt Treatment**
Michihisa FUKUMOTO (Akita University, Japan)

16:50-17:10 **I-F0483** **[Invited] In Situ Micro Cantilever Beam Bending Tests to Explore the Adhesion Strength of Cr Coatings on Zry – 4**
Nan Li (Los Alamos National Laboratory, USA)

17:10-17:30 **I-F0946** **[Invited] Innovative Manufacturing for Clean Energy Applications by Thermal Spray Technology**
Surinder Singh (Swinburne University of Technology, Australia)

# Characterization of a Cobalt-Chromium-Molybdenum Alloy Subjected to Surface Mechanical Attrition Treatment

**Gwénaëlle Proust**[1], Cecilie Funch[2], Lucas Brasileiro[3], Zhidan Sun[4], Delphine Retraint[5]

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## Abstract

Surface Mechanical Attrition Treatment (SMAT) is a severe plastic deformation process derived from shot peening that enhances the surface properties and performance of a material by creating a nanostructured layer on the top surface of the material. SMAT has been shown to improve mechanical properties of materials such as hardness, strength, fatigue life and wear resistance for a large range of metallic alloys. The process was applied to a CoCrMo alloy used in biomedical applications with the aim to improve its mechanical properties. Two different SMAT treatments were realized on the alloy. Changes in the microstructure due to SMAT were characterized using transmission electron microscopy, electron backscatter diffraction and transmission Kikuchi diffraction. It was observed that the formation of the nanostructured layer was driven by phase transformation; the alloy transforming from an fcc to an hcp phase during SMAT. The microstructure changes can explain the improved hardness and fatigue life measured on the SMATed samples.

*Keywords: Co-Cr alloys, Surface treatment, Shot peening, SMAT, Microscopy*

# Formation of Porous Ni-Pt Alloy using the Molten Salt Treatment

**Michihisa Fukumoto[1],** Maya Satou[2], Ryu Takahashi[3], Hiroki Takahashi[4]

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## Abstract

Recently, it is desired to highly active electrode materials for alkaline water hydrolysis to produce hydrogen in order to achieve sustainable society. As a cathode material, Ni-Pt alloy porous layer was formed by electrodepositing Pt on Ni substrate sample, followed by Al-depositing and Al-dissolving at high temperature. The Pt was electrodeposited using an aqueous solution as an electrolyte, and the Al-depositing and Al-dissolving were conducted using a molten salt as the medium. The molten salt used was NaCl-KCl- 3.5 mol%$AlF_3$. A Ni-Pt-Al alloy layer was formed when Al was electrodeposited after Pt electrodeposition. It was found that the porous surface of Ni-Pt was finer than that of Ni. Furthermore, it was clarified that the lower the electrodeposition potential of Al, the thicker the Ni-Pt alloy porous layer. Ni-Pt alloy was formed uniformly when the treatment temperature in the molten salt was high. The cathode polarization curve was measured in KOH solution, and the amount of hydrogen gas was determined when water electrolysis was performed at constant voltage with a hydrogen detection gas sensor using a tubular proton conductor ($CaZr_{0.9}In_{0.1}O_{3-a}$). As a result, the amount of hydrogen generated sharply increased due to the porous treatment with molten salt. Therefore, it was clarified that this method is effective for preparing hydrogen generation electrode.

*Keywords: Hydrogen electrode; Molten Salt; Ni-Pt alloy; Porous layer; Hydrogen sensor*

**T**his work was primarily supported by the Iketani Science and Technology Foundation, ISTF, Japan.

# In Situ Micro Cantilever Beam Bending Tests to Explore the Adhesion Strength of Cr Coatings on Zry - 4

**Nan Li[1],** Dongyue Xie[2], Hyosim Kim[3], Tyler Dabney[4], Ben Eftink[5], Kumar Sridharan[6], Tim Graening[7], Andrew Nelson[8], Saryu Fensin[9], Stuart Maloy[10]

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## Abstract

Due to the combined advantage of low thermal neutron absorption coefficient, good corrosion resistance in high temperature water, and satisfying mechanical properties, zirconium alloys have been widely used as a fuel cladding material in light water reactors (LWRs). Following the Fukushima-Daiichi accident in 2011, increasing concerns were triggered on the oxidation and hydrogen gas generation issues of Zr alloys under severe accident environments. Significant effort has been developed to apply Cr coatings to suppress water corrosion at elevated temperatures due to their extraordinary corrosion resistance, high melting point, good strength, high hardness, and good wear resistance. Here, two types of coating methods have been applied: (i) High Power Impulse Magnetron Sputtering (HiPIMS) to deposit a 6-micron Cr coating at Oak Ridge National Laboratory; (ii) cold spray to deposit a 50-micron Cr coating from the University of Wisconsin-Madison. Micro scale cantilever beams with a pentagonal cross section have been fabricated inside the Cr coating region. In situ bending tests were performed using a PI-89 Pico-indent system (Hysitron/Bruker Inc., USA) inside a scanning electron microscope (SEM). The beam failed brittlely at the interface of coatings and the Zry-4 plate. The adhesion strength correlated with the the fracture stresses of the Cr coatings on the Zry - 4 plates has been estimated.

*Keywords: Cr coatings; cantilever beam bending; radiation damage*

# Innovative Manufacturing for Clean Energy Applications by Thermal Spray Technology

**Surinder Singh[1],** Nonthapat Nawbuntud[1], Christopher C. Berndt[1], M. Nagini [2], B.S. Murty[2], Andrew S. M. Ang[1,]

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**Abstract**

All solid-state thin film battery (ASSTB) technology has gained substantial attention due to its longer lifespan and greater safety compared to conventional liquid electrolyte-based lithium-ion batteries. Diverse strategies, including materials optimisation and vacuum based fabrication techniques, have been explored to achieve stable and high energy capacity (>372 mAh/g) ASSTBs. However, the materials and fabrication methods to fabricate ASSTB components such as the solid electrolyte, anode, and cathode, are typically expensive, characterized by slow deposition rate and yield mostly amorphous coatings that demand post-processing to enhance performance.

The key to commercialize ASSTBs is to explore new functional materials and fabrication methods. In this context, liquid feedstock thermal spraying techniques relying on suspensions as feedstock provide technical as well as economic advantages. This proof-of-concept study discusses deposition of (i) $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$ (NMC111) as the cathode, (ii) a high entropy oxide based anode, and (iii) $Li_7La_3Zr_2O_{12}$ (LLZO) as the electrolyte. Powders of all the above chemistries were procured and oxides were prepared using high energy ball milling. Further, suspensions were prepared in-house using additives to enhance suspension stability. The influence of spray variables on density, crystallinity and microstructure has been assessed to develop process-structure-performance relationship. The electrochemical performance of these ASSTB components have been evaluated and promote promising behaviour.

*Keywords: Thermal spray; coatings, Li-ion batteries, suspension, high-entropy oxides, LLZO.*

Acknowledgement: This work has been supported by the Australian Research Council (ARC). The ARC Training Centre in Surface Engineering for Advanced Materials, SEAM, has been funded under Award IC180100005. Additional support has derived from industrial, university and other partners.

# Technical **Oral Session _ Session 6**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 6 (G6)** **16:00 - 18:00, Nov. 21**

**Chair :** Jin-Wook Lee (Sungkyunkwan University) 303A, 3F

16:00-16:20 **I-G0297** **[Invited] Critical Factors Affecting Fill Factor in All Polymer Solar Cells**
Hyung Do Kim (Kyoto University, Japan)

16:20-16:40 **I-G1104** **[Invited] Toward efficient, stable and reproducible metal halide perovskite solar cells**
Jin-Wook Lee (Sungkyunkwan University, Korea)

16:40-17:00 **I-G1133** **[Invited] Phase Stabilization Strategies for Efficient Perovskite Solar Cells**
Peng Chen (The University of Queensland, Australia)

17:00-17:15 **O-G0018** **Recent progresses and remaining issues on the catalyst layer design strategy for high-performance proton exchange membrane fuel cell with further reduced Pt loadings**
Xiang Deng (Sinosteel Nanjing Advanced Materials Research Institute Co., Ltd., Australia)

17:15-17:30 **O-G0154** **Cu doped NiFe double-layered hydroxide electrocatalyst for oxygen evaluation reaction in anion exchange membrane water electrolysis**
Debabrata Chanda (Kumoh National Institute of Technology, Korea)

17:30-17:45 **O-G0840** **Synchronous bi-modulation by nanoclusters and single atoms for high-efficient oxygen reduction electrocatalysis**
Ying Zhang (Jilin University, China)

17:45-18:00 **O-G0841** **CeO2 nanoparticles decorated on porous Ni-Fe bimetallic phosphide nanosheets for high-efficient overall water splitting**
Li Du (Jilin University, China)

# Critical Factors Affecting Fill Factor in All Polymer Solar Cells

**Hyung Do Kim**[1]

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**Abstract**

It is substantially desirable to realize a high fill factor (FF) even with thick active layers that yield large short-circuit current density ($J_{SC}$) for highly efficient all polymer solar cells. This is, however, typically restricted by charge recombination in competition with charge collection. Thus, of the particular importance is to overcome a tradeoff relation between FF and $J_{SC}$. In this talk, I will address some of the factors determining this phenomenon in these devices consisting of donor- and acceptor-conjugated polymers and how these impact upon FF based on the recombination kinetic parameters measured by transient optoelectronic techniques. I will start by introducing four kinds of polymer solar cells based on blends of polymer donors with different crystallinities and polymer acceptors with a naphthalene diimide unit (N2200). In these systems, I will discuss how crystallinity of polymer donors impacts on bimolecular recombination. I will then go on to focus on polymer solar cells based on crystalline donor polymers with different side chains and an N2200 acceptor polymer to discuss how charge collection and recombination impact on FF in thick films. The impact of morphologies on charge recombination, and thus on FF, will be addressed for all the solar cells studied. Throughout my talk, I will try to highlight the critical factors affecting FF and how we can achieve highly efficient polymer solar cells.

*Keywords: All polymer solar cells, Fill factor, Crystallinity, Bimolecular recombination, Langevin recombination*

# Toward efficient, stable and reproducible metal halide perovskite solar cells

**Jin-Wook Lee[1]**

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**Abstract**

Metal halide perovskite solar cells (PSCs) have been spotlighted as a promising next-generation solar cell. Nevertheless, several challenges remain unresolved toward commercialization. One of the major challenges is their poor operational stability originating from abundant mobile defects. In this presentation, I will first report our strategies to mitigate detrimental effects of the defects. We identified the side effects caused by conventional defect passivation processes, which seriously degrade performance and stability of the perovskite solar cells. We propose a possible solution for minimizing the side effects to maximize attainable performance and stability of the devices. In second part of the presentation, I will discuss the reproducibility issue of the PSCs. Reproducible fabrication of PSCs is a critical consideration for market viability and practical commercialization. In this work, we unravel the critical function of atmospheric humidity to regulate the crystallization and stabilization of formamidinium lead triiodide ($FAPbI_3$) perovskites. We demonstrate that the humidity content during processing underlies profound variations in perovskite stoichiometry, thermodynamic stability, and optoelectronic quality.

*Keywords: perovskite solar cells, stability, reproducibility, defect, humidity*

# Phase stabilization strategies for efficient perovskite solar cells

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**Abstract**

The recent decade has witnessed the rapid increase in the power conversion efficiency of metal halide perovskite solar cells (PSCs) from 3.8% to certified 25.7%. Despite their success in achieving intriguing photovoltaic performance, the inferior phase stability of PSCs against external stimuli (e.g. moisture and UV light) remains a critical hurdle for their further large-scale applications. Herein, we introduced innovative strategies, including interfacial engineering,[1-2] surface ligand decoration,[3] and material composition,[4] to stabilize the photoactive phase and simultaneously passivate surface defects of perovskites for optoelectronic applications. By rational design on interfacial and surface engineering, the fabricated PSCs delivered a champion power conversion efficiency of 23.89%, which can be retained 90% after aging in a humid atmosphere (relative humidity level 60%) for 1,000 hours. Besides, the synthesized perovskite-metal organic framework composites showed excellent photoluminescence stability against water immersion for 10,000 hours, which can serve as a desirable encapsulation technique for perovskite optoelectronics in the future.

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**Submitting to the Symposium G: Materials for Energy Storage and Generation**

*Keywords: perovskite solar cells, phase stability, interfacial engineering, composite materials, metal-organic frameworks*

# Recent progresses and remaining issues on the catalyst layer design strategy for high-performance proton exchange membrane fuel cell with further reduced Pt loadings

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## Abstract

This presentation reports our recent investigation and work on the catalyst layer design strategy for high-performance proton exchange membrane fuel cell (PEMFC). Specifically, the motivation towards the further reduced Pt loadings by applying new electrode design strategies is firstly introduced from both the historical and mechanism deductions. Then, the recent developments on the catalyst layer designs belonging to different classifications are summarized with their respective merits. In particular, we will report our work on the novel design of a bi-functional layer consisting of vertically aligned carbon nanotubes (VACNTs) and nanoparticles of Pt-Co catalysts (Pt-Co/VACNTs) for high-performance PEMFCs. Readily prepared by a two-step process, the Pt-Co/VACNTs layer with a hydrophilic catalyst-loaded side and a hydrophobic gas diffusion side enables a PTFE-free electrode structure with fully exposed catalyst active sites and superior gas-water diffusion capability. This remarkable design of VACNTs-based catalyst with dual functionalities enables much lower Pt loading, faster mass transport, and higher electrochemical performance and stability. Further, the preparation procedure can be easily scaled up for low-cost fabrication and commercialization. This unique bi-functional layer structure as proposed in this work may offer new insights into the development of integrated cell configuration with multi-functionalities. Finally, we will discuss the critical issues remained on these low Pt-loaded electrodes with the possible solutions in the near future.

*Keywords: Catalyst layer design, Reduced Pt loading, Proton exchange membrane fuel cells (PEMFC), Vertically aligned carbon nanotube arrays(VACNTs)*

# Cu doped NiFe double-layered hydroxide electrocatalyst for oxygen evaluation reaction in anion exchange membrane water electrolysis

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## Abstract

Dedicated design of nanocages architectures for oxygen evaluation reaction (OER) electrocatalysts is an important game changing strategy to accelerate overall water splitting kinetics. In this study, we adopt a unique facile route to prepare copper-mediated layered double hydroxide NiFe (CuNiFe-LDH) nanocapsules architectures for excellent oxygen evaluation reaction (OER) overpotential ($\eta$) of 201mV at current density ($j$) 10 mA $cm^2$. This result demonstrate that the electronic coupling and coordination of Cu ions stabilize the initial structures of the conductive NiFe MIL-88A metal-organic frameworks (MOFs). Moreover, a photovoltaic electrochemical-water splitting (PV-EC) device without wiring has been fabricated with CuNiFe-LDH/Ni mesh (NM) OER electrode, demonstrating direct solar to hydrogen production (STH) of 11.08 % with 20 h stable operation. Also, exhibits excellent OER activity for anion exchange membrane water electrolysis (AEMWE) with $j$ of 974 mA $cm^{-2}$ at 1.85 V. This study provides information on new MOF based architectures for electrochemical applications.

# Synchronous bi-modulation by nanoclusters and single atoms for high-efficient oxygen reduction electrocatalysis

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## Abstract

Developing single-atom catalysts with robust performance for oxygen reduction reaction (ORR) is of paramount importance, whereas their unsatisfactory intrinsic activity remains a significant challenge. Herein, density functional theory simulation indicates that the synchronous bi-modulation by Co nanoclusters and Zn single atoms ($ZnN_4$) can increase Co active centers' electron density, thus improving the intrinsic activity of Co single-atom ($CoN_4$) sites. Inspired by these findings, a multiscale catalyst with highly-dispersed Co/Zn metal atoms and nanoclusters anchored on a porous N-doped carbon skeleton has been successfully synthesized. The resultant $Co_1/Zn_{20}$-N-C-200 exhibits remarkable ORR performance with a positive half-wave potential ($E_{1/2}$ = 0.89 V), outstanding methanol tolerance, and superior stability in alkaline media, outperforming a majority of nonprecious metal-based catalysts and the benchmark Pt/C catalyst in some aspects. $Co_1/Zn_{20}$-N-C-200 also achieves high open-circuit voltage of 1.47 V and power density of 116 mW $cm^{-2}$ when applied in the self-made Zn-air battery.

*Keywords: Bi-modulation; Oxygen reduction reaction; Single atoms; Nanoclusters; DFT simulation*

# $CeO_2$ nanoparticles decorated on porous Ni-Fe bimetallic phosphide nanosheets for high-efficient overall water splitting

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## Abstract

Transition-metal phosphides have been widely explored as water splitting electrocatalysts. However, they generally possess poor long-term stability during the water electrolysis, and their catalytic activity is still desirable to be further improved. Herein, a self-supported electrode was designed and prepared for the first time with $CeO_2$ nanoparticles decorated on porous Ni-Fe bimetallic phosphide nanosheets, which were grown on high-conductivity Ni foam. Owing to the strong electronic interactions between the heterostructure interfaces and the introduction of oxygen vacancies, such an electrode displays outstanding oxygen evolution reaction performance with a low overpotential of 188 mV at 10 mA $cm^{-2}$ and the electrolyzer using the electrode as both cathode and anode exhibits a low cell voltage of 1.54 V at 10 mA $cm^{-2}$. Furthermore, density functional theory simulations indicate that oxygen vacancy engineering is an effective strategy for adjusting the electronic structure of catalysts and the adsorption of reaction intermediates.

*Keywords: $CeO_2$; bimetallic phosphide; oxygen vacancy; water splitting; DFT simulations*

# Technical **Oral Session _ Session 6**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 6 (H6)** **16:00 - 17:40, Nov. 21**

**Chair :** Yu Shiratsuchi (Osaka University) 303B, 3F

16:00-16:30 **K-H0316** **[Keynote] Processing for IV-VI 2D semiconductors based on thermodynamics**
Yoshitaro Nose (Kyoto University, Japan)

16:30-16:50 **I-H0279** **[Invited] Emerging Sb- and Ge- based layered tellurides for electronic device application**
Yuta Saito (National Institute of Advanced Industrial Science and Technology, Japan)

16:50-17:10 **I-H0466** **[Invited] Engineering the filamentary threshold switching response of NbOx**
Shimul Kanti Nath (University of New South Wales, Australia)

17:10-17:25 **O-H0246** **TM-O-Te system for new class of As- and Se-free OTS materials**
Shogo Hatayama (National Institute of Advanced Industrial Science and Technology, Japan)

17:25-17:40 **O-H1087** **One-dimensional core-sheath Sn/SnOx derived from MAX phase for microwave absorption**
Feiyue Hu (Southeast University, China)

# Processing for IV-VI 2D semiconductors based on thermodynamics

**Yoshitaro Nose**[1]

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## Abstract

2D semiconductors such as graphene and transition metal dichalcogenides have attracted much attention in the viewpoints of both fundamental science and practical applications. These materials show specific physical properties due to their strong anisotropy in lattice structure. Monochalcogenides consisted with IV and VI group elements also have 2D structure, so-called puckered structure, and are potential for photovoltaics, thermoelectric devices, piezoelectric devices, and transistors. For practical applications, it is required to develop efficient method for fabrication and the way to control properties. Taking one of IV-VI materials SnS as an example, a condition window for preparation is quite narrow as derived from thermodynamics, namely the range of chemical potentials of constituent elements is limited from an equilibrium point of view.

In our group, a novel processing route to obtain single-phase SnS has been proposed. The vapor pressure of SnS is much higher than that of Sn, and therefore SnS can be separated as a vapor from SnS/Sn composites, in which chemical potentials are thermodynamically determined. Specimens with any shapes such as bulk crystals, thin films, and powders can be prepared. Chemical potential is also a factor to control point defect formation, leading to carrier density. Utilizing of composites gives advantage for the control of chemical potentials, including extrinsic doping.

In the presentation, our concept and some topics related to single crystal fabrication and carrier type control are introduced and discussed.

*Keywords: vapor phase growth, chemical potential, doping in semiconductors, single crystal*

# Emerging Sb- and Ge- based layered tellurides for electronic device application

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## Abstract

The Ge-Sb-Te ternary alloy is the most common phase-change material, which has been used for rewritable optical discs as well as non-volatile memory applications. Here, we present two binary tellurides in this ternary system, namely, $Sb_2Te_3$ and $GeTe_2$. $Sb_2Te_3$ is a layered material and known as the representative topological insulator. $Sb_2Te_3$ has a band gap of about 0.2–0.3 eV and easily becomes a degenerated p-type semiconductor. Due to the presence of Te-terminated van der Waals surface and the semimetal-like band structure, we show that $Sb_2Te_3$ can be a good contact electrode for monolayer $MoS_2$ MOSFET [1]. $GeTe_2$ does not exist in nature as it spontaneously decomposes into the stable GeTe and Te in the equilibrium state. This metastable phase can be formed only in thin film form by crystallization of the amorphous film. We found that $GeTe_2$ shows a layered structure of Te-Ge-Te atomic layer stacking similar to transition metal dichalcogenides. Moreover, this metastable layered $GeTe_2$ exhibited the semiconducting behavior, which is a promising candidate for novel electronic devices [2]. These two examples suggest that layered tellurides possess a large potential for significantly improving the future electronic devices.

[1] W. H. Chang et al., *Adv. Electro. Mater.* 2201091 (2023).
[2] Y. Saito et al., *Mater. Horiz*. doi.org/10.1039/D2MH01449A (2023).

*Keywords: layered telluride, $Sb_2Te_3$, $GeTe_2$, transistor, contact.*

# Engineering the filamentary threshold switching response of $NbO_x$

**Shimul Kanti Nath**[1], Sanjoy Kumar Nandi[2], Assaad El-Helou[3], Shuai Li[2], Thomas Ratcliff[2], Perter Raad[3], Robert G. Elliman[2]

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## Abstract

Two-terminal metal-oxide-metal memristors exhibit characteristic non-volatile and volatile resistance changes when subjected to external stimuli and have received significant interests for application in neuromorphic computing, memory technology and security. The resistance changes are typically observed after an initial electroforming process that forms a filamentary conduction path which subsequently governs the device characteristics. Knowledge about the structure, composition and spatial distribution of these filaments is essential for a full understanding of device response and effective modelling and optimisation of associated devices. Additionally, understanding the factors governing the switching modes and parameters are necessary for achieving reliable device response with tuneable parameters which is crucial for practical applications.

This presentation summarizes our recent works on filamentary threshold switching in niobium-oxides ($NbO_x$) and discusses pathways to engineer the device responses by employing numerous techniques, including electrical testing, lumped element modelling and in-situ thermo-reflectance imaging [1-5]. At first, a simple means of detecting and spatially mapping conductive filaments is introduced, and the utility of this technique is demonstrated to identify distinct modes of electroforming in low- and high-conductivity $NbO_x$ films. Then, the role of oxide conductivity, temperature dependence of device resistance, choice of electrodes and metal/oxide interface reactions on the post-forming characteristics is discussed.

[1] Nath et al. Applied Physics Letters, 2019 (114), 062901

[2] Nandi et al. ACS Applied Materials & Interfaces, (2021)13(2), 2845

[3] Nath et al. ACS Applied Materials & Interfaces, 2020 (12), 8422

[4] Nath et al. Nanoscale 2023 (15), 7559

[5] Nath et al. Nanotechnology, (2020) 31(23), 235701

*Keywords: Oxides, threshold switching, filaments, device engineering, interfacial phenomena*

# TM-O-Te system for new class of As- and Se-free OTS materials

**Shogo Hatayama**[1] and Yuta Saito[1]

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## Abstract

Ovonic threshold switch (OTS) materials are regarded as a key material for the selector function in Xpoint architecture. These materials exhibit threshold-type current-voltage characteristics, enabling ON (low resistance) and OFF (high resistance) volatile switching, which serves as a selector function. Most OTS materials contain good glass-forming elements such as Se and Te, with As to form rigid amorphous networks. However, due to their toxicity, there is a strong demand for As- and Se-free OTS materials. In this study, we propose the transition metal (TM)-O-Te systems as a new class of OTS materials. The amorphous TM-based chalcogenides generally exhibit low electrical resistivity. Therefore, we aimed to enlarge the band gap ($E_g$) by alloying with O to overcome the limitation of insufficient OFF state resistivity. As a candidate TM-O-Te system, Hf-O-Te ternary amorphous films were investigated. Although the Hf oxide is an insulator with an $E_g$ of around 5 eV, the $E_g$ value was found to decrease with increasing Te content. The $Hf_{0.24}O_{0.55}Te_{0.21}$ film with an $E_g$ of 1.0 eV exhibits a selector function. These findings provide a way to develop novel As- and Se-free OTS materials [1]. In the presentation, we will demonstrate the results of other TM-O-Te system.

[1] S. Hatayama, Y. Saito, and N. Uchida, *APL Mater*. **10**, 011106 (2022).

*Keywords: Selector function, Amorphous chalcogenide, OTS material, Transition metal, Non-linear I-V.*

# One-dimensional core-sheath Sn/$SnO_x$ derived from MAX phase for microwave absorption

**Feiyue Hu[1],** Zhihua Tian[2], Wenwen Sun[3], Peigen Zhang[4*], ZhengMing Sun[5*]

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## Abstract

One-dimensional (1D) metals are highly conductive and tend to form networks that facilitate electron hopping and migration. Hence, they have tremendous potential as microwave-absorbing (MA) materials. Traditionally, 1D metals are mainly precious metals such as gold, silver, nickel, and their preparation methods often have low yield and are not environmentally friendly, which has limited the exploration in this area. Herein, the unique nanolaminate structure and chemical bond characteristics of $Ti_2SnC$ MAX phase are successfully taken advantages for large-scale preparation of Sn whiskers, and then, core-sheath Sn/$SnO_x$ heterojunctions are obtained by simply annealing at different temperatures. The heterojunction annealed at 500 °C possesses superior MA performance with an effective absorption bandwidth of 5.3 GHz (only 1.7 mm) and a minimum reflection loss value of −51.97 dB; its maximum radar cross section (RCS) reduction value is 29.59 dB $m^2$, confirming its excellent electromagnetic wave attenuation ability. Off-axis electron holography is used to visually characterize the distribution of charge density at the cylindrical heterogenous interface, confirming the enhanced interfacial polarization effect. Given the diversity of MAX phases and the advantages of the fabrication method (e.g., green, inexpensive, and easily scalable), this work provides significant guidance for the design of 1D metal-based absorbers.

*Keywords: Sn/SnOx heterojunctions; $Ti_2SnC$ MAX phase; Microwave absorption; Interfacial polarization*

[1] **F.Y. Hu,** B.B. Fan*, Rui Zhang, et al. Tailoring electromagnetic responses of delaminated $Mo_2TiC_2T_x$ MXene through the decoration of Ni particles of different morphologies. Chemical Engineering Journal, 2022, 440: 135855.
[2] **F.Y. Hu,** B.B. Fan*, Rui Zhang, et al., et al. Ultrabroad band microwave absorption from hierarchical $MoO_3/TiO_2/Mo_2TiC_2T_x$ hybrids via annealing treatment. Journal of Advanced Ceramics, 2022, 11(9): 1466-1478.
[3] **F.Y. Hu,** B.B. Fan*, Rui Zhang, et al. Synthesis and electromagnetic wave absorption of novel $Mo_2TiC_2T_x$ MXene with diverse etching methods. Journal of Materials Science, 2022, 57: 7849-7862.
[4] **F.Y. Hu,** B.B. Fan*, Rui Zhang, et al. Green rapid synthesis of $Cu_2O$/Ag heterojunctions exerting synergistic antibiosis. Chinese Chemical Letters, 2022, 33(1): 308-313.

# Technical **Oral Session _ Session 6**

## **Symposium I :** Biomaterials and Soft Materials and their Application

**Biomaterials and Soft Materials and their Application 6 (I6)** **16:00 -18:05, Nov. 21**

**Chair :** Luning Wang (University of Science and Technology Beijing) 400, 4F

16:00-16:30 **K-I1092** **[Keynote] Biodegradable structures based on magnesium alloys for osteosynthesis in medicine - development and prospects for use**
Nikolay Redko (Moscow State University, Russia)

16:30-16:50 **I-I0775** **[Invited] Two-Dimensional Nanoassemblies from Plasmonic Matryoshka Nanoframes**
Qianqian Shi (Monash University, Australia)

16:50-17:05 **O-I0415** **Fabrication of polypropylene nanoplastics via thermal oxidation reaction for human cells responsiveness studies**
Masaya Yamamoto (Tohoku University, Japan)

17:05-17:20 **O-I0237** **Model Samples of Nano-sized Plastics**
Ikuna Kanehara (Shibaura Institute of Technology, Japan)

17:20-17:35 **O-I0712** **An implantable and wireless drug delivery device for the enhancement of drug efficacy**
Sung-Geun Choi (Seoul National University, Korea)

17:35-17:50 **O-I0419** **Polymorphism control of Glycine crystals by Terahertz wave irradiation**
Mana Kusama (Shibaura Institute of Technology, Japan)

17:50-18:05 **O-I0236** **Pyroelectric effect of grown Triglycine sulfate crystals**
Kazuma Iwasaki (Shibaura Institute of Technology, Japan)

# Biodegradable structures based on magnesium alloys for osteosynthesis in medicine - development and prospects for use

**Nikolay Redko**[1], Alexey Drobyshev[2], Kwang Seon Shin[3], Alexander Komissarov[4], Zaira Gurganchova[5]

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Several million people annually suffer from bone fractures caused by accidents (car accidents, industrial disasters, etc.) or various diseases. In a large part of these operations (up to 50%), titanium structures and elements fixing bone tissue are used. Currently, active developments are underway on the use of products from various bioresorbable magnesium alloys in medicine and veterinary medicine. Magnesium-based alloys developed in recent years have shown improved corrosion resistance and mechanical properties and are promising materials for making biodegradable, biocompatible metal implants.

Wistar rats, where the level of resorption of pins installed in the femur at stages of 1, 3 and 6 months was assessed. The rate of resorption was assessed according to the data of radiation methods of research, histological assessment, SEM and EDX. The results obtained indicate a significant bioresorption of the magnesium pin at 3 months and complete degradation 6 months after the operation.

According to the X-ray methods of examination, it is determined that the established pins gradually degrade in the period from 1 to 6 months, reducing their average density. At a period of 6 months, residual fragments of the established pins were determined only on micro-CT. Histological assessment of the implantation zone indicates the gradual filling of the implant bed with fibrous tissue with an abundance of capillaries and a ring-shaped area of compact mature bone. There is no inflammatory infiltration. Bone formation after implantation demonstrates osteointegration and therefore good biocompatibility with the surrounding bone tissue.

*Keywords: biodegradable materials, osteosynthesis, magnesium alloys, bioresorption*

# Two-Dimensional Nanoassemblies from Plasmonic Matryoshka Nanoframes

**Qianqian Shi,[1]** Runfang Fu,[1] Debabrata Sikdar,[2] Tharaka Perera,[3] Anthony S. R. Chesman,[4] Zijun Yong,[1] Yan Lu,[1] Yiyi Liu, [1] Zhirui Guo, [1] Shu Gong, [1] Malin Premaratne, [3]and Wenlong Cheng[1]*

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**Abstract**

Two-dimensional (2D) plasmonic nanoassemblies are programmable ultrathin materials that one can, in principle, adjust the size and shape of their constituent building blocks to fine-tune collective optical, electrical, and mechanical properties. In this talk, I will introduce a new 2D nanoassembly from structurally complex plasmonic building blocks, namely, matryoshka-like gold (Au) nanoframes. Using a seed-mediated alternating deposition of Au and silver (Ag) elements in conjunction with a selective etching process, we obtain monodisperse matryoshka-like Au nanoframes with a nesting number (Nn) of up to 5. A cubic nanoframe displays dominant intraplasmonic coupling attributed to bonding and antibonding dipolar modes, which shift to blue and red, respectively, with an increased Nn. Combined with polystyrene (PS) ligand exchange and drying-mediated self-assembly, the approach mentioned above can be used to produce 2D plasmonic matryoshka nanoassemblies. Both experimental and simulation results demonstrate the presence of intra- and inter-ridge plasmonic coupling in the nanoassemblies. The 5-nested nanomatryoshka assemblies exhibit a Raman enhancement 14-fold greater than those with 1-nested cubic nanomatryoshka, demonstrating the dominant intraridge hot spot effects. Taking advantage of interparticle distance-dependent optical transparency of 2D matryoshka nanoframe assemblies, we further demonstrate temperature-enabled encryption/decryption using thermos responsive polymers.

Topic area: Symposium I. Biomaterials and Soft Materials and their Application.

*Keywords: plasmonic, 2D nanoassemblies, nanoframe, self-assembly, SERS.*

# Fabrication of polypropylene nanoplastics via thermal oxidation reaction for human cells responsiveness studies

**Masaya Yamamoto[1,2],** Suphatra Hiranphinyophat[1], Tomoki Hiraoka[1], Naoto Washihira[1], Akio Kishida[3], Sho Fujii[4], Mako Kobayashi[1], Tadao Tanabe[5], Tsuyoshi Kimura[3]

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## Abstract

With the current worldwide increasing use of plastics, nanoplastics (NPs) have become a global threat to environmental and public health concerns. Among plastics, polypropylene (PP) is widely used for industrial and medical applications. Owing to the lack of validated detection methods and standard materials for PP NPs, understanding of the impact of PP NPs on the environmental and biological systems is still limited. Here, isotactic polypropylene (iPP) was fabricated into micro/nanosized (OPPMPs/OPPNPs) via a thermal oxidation approach by using hydrogen peroxide as a solvent under various heating temperatures, and the resulting OPPMPs/OPPNPs were evaluated in terms of the size distribution, surface functional groups, morphology, and thermal property. Using the well-characterized PP NPs, their concentration-dependent cytotoxicity was examined with human colon carcinoma cell lines (Caco-2). The average diameters of OPPMPs/OPPNPs decrease with increasing the reaction temperature. The obtained OPPNP at 175 degrees Celsius (OPPNP175) was spherical in shape and rough surface with size distributions of approximately 144.0 ± 0.1 nm. A significant increase in the carbonyl content of the oxidized product was confirmed by FTIR and XPS analysis. Caco-2 cells were exposed to OPPNP175 in a dose-dependent manner, and cytotoxic concentrations showed that a significant loss of cell viability occurred in the presence of 500 μg/mL. Taken together, this study provides a fundamental approach for the fabrication of nanoplastics for the urgently demanded in vitro and in vivo studies to assess the potential impact of nano-sized plastics on biological systems.

*Keywords: nanoplastics, thermal oxidation, degradation, polypropylene, cytotoxicity*

# Model Samples of Nano-sized Plastics

**Ikuna Kanehara**[1], Hiromasa Yamashita[2], Sho Fujii[3], Tsuyoshi Kimura[4], Masaya Yamamoto[5], Tadao Tanabe[6]

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## Abstract

Plastics in the environment can be fragmented into nano-sized particles (NPs) by UV irradiation or mechanical means. The morphological characteristics of NPs have been reported to be different from those of particulate samples used for interactions with biological systems and toxicity studies. In this study, model samples simulating NPs dispersed in the environment were artificially prepared by laser ablation.

NPs were produced by irradiating a 50 μm thick low-density polyethylene (LDPE) film with a UV (266 nm) nano-second laser at a repetition rate of 10 Hz to locally break σ bonds. The LDPE film was placed in a cell filled with ultra-pure water in an environment as free of solvent residue and surfactants as possible. The particle size of NPs was measured by Dynamic Light Scattering (DLS), and the shape of NPs was confirmed by field emission scanning electron microscopy (FE-SEM). Particle size measurement by DLS showed that particles with an average size of 180 nm after 12 hours of laser irradiation, and observation of particle shape by FE-SEM showed not only independent particles but also some agglomerated states (Fig.1). Laser ablation has been used to produce NPs that can be used as model samples for ecological interactions and toxicological studies.

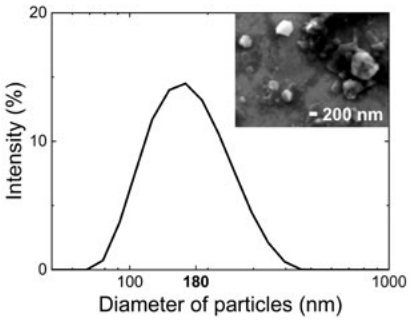



Fig.1 Particle size distribution by scattering intensity and FE-SEM observation image (upper right)

In this presentation, we will discuss whether nanosecond laser ablation can generate NPs and their material properties, including the results of other measurements. This research is a result of JST-CREST (Integrated understanding of degraded nanomaterials coexisting in environmental and biological cycles).

*Keywords: nano-plastics, laser ablation, nano-second laser, dynamic light scattering, field emission scanning electron microscope*

# An implantable and wireless drug delivery device for the enhancement of drug efficacy

**Sung-Geun Choi**[1], Seongchan Kim[2], Joon-Woo Kim[3], Myung-Kyun Choi[4], Jieun Han[5], Jeonghyun Kim[6], Hyojin Lee[7], Seung-Kyun Kang[8]

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## Abstract

The previous generation of implantable drug delivery systems used convection or diffusion of drug solutions to localize the drug effect. However, each method has clear limitations. Convection methods can cause incorrect delivery to normal tissue due to the flow of drug solution, while diffusion methods cannot control the rate of drug release. Furthermore, these methods focus only on exposing drugs to the surface of the disease site, making it difficult to target drugs to lesions located in deeper tissues. We have developed a wirelessly controlled electrical drug delivery system to enhance drug delivery controllability and drug penetration into tissue. The device uses an bipolar membrane as a release control membrane. The bipolar membrane can control the rate of drug release under an electric field with bias direction and amplitude. This electrical drug delivery method can concentrate drugs in clusters by transporting only solutes. In addition, the ion current passing through the tissue can induce drugs to reach deeper tissues, increasing the bio-distribution of drugs. The wirelessly controlled electrical drug delivery system can improve drug efficacy by allowing for the electrical control of drug release according to an individual drug schedule and by distributing drugs throughout pathological tissues.

*Keywords: Drug delivery system, bipolar membrane, biomaterial, iontophoresis, ion transport*

# Polymorphism control of Glycine crystals by Terahertz wave irradiation

**Mana Kusama**[1], Kazuma Iwasaki[2], Sho Fujii[3], Tsuyoshi Kimura[4], Masaya Yamamoto[5], Tadao Tanabe[6]

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## Abstract

Terahertz waves are being applied to the evaluation of physical properties, such as the identification of plastic materials and nondestructive testing of rebar in concrete. The energy of terahertz waves corresponds to intermolecular interactions on which the material evaluation is based. In contrast to the evaluation, the terahertz waves for manufacturing have not yet been developed. One of the phenomena involving intermolecular interactions is molecular crystallization. Then we were curious whether terahertz irradiation would affect the crystallization. The purpose of this study is to utilize terahertz waves for crystal structure control by irradiating terahertz waves during solution growth of glycine crystals.

Two beakers containing 50 g of saturated glycine solution are prepared. One is irradiated with 40 GHz electromagnetic waves. Crystals of glycine are obtained by spontaneous drying. The two types of crystals obtained from each beaker are analyzed by X-ray diffraction (XRD).

The XRD pattern showed that the crystals without the irradiation were γ-glycine which is the most stable crystalline polymorph of glycine at room temperature. The crystals with the irradiation were also γ-type glycine at 40 hours of growth time (Fig. 1). However the XRD pattern contained both α- and γ-type features at 48 hours. Then at 89 hours the γ-type was disappeared, and it became α-type glycine.

These results indicate that the irradiation of 40 GHz electromagnetic waves induce crystal phase transition of glycine from γ-type to α-type. It is considered that the longer the growth (irradiation) time, the higher the dislocation rate from γ-type to α-type.

*Keywords: Terahertz wave, glycine, crystal growth, polymorphism control*

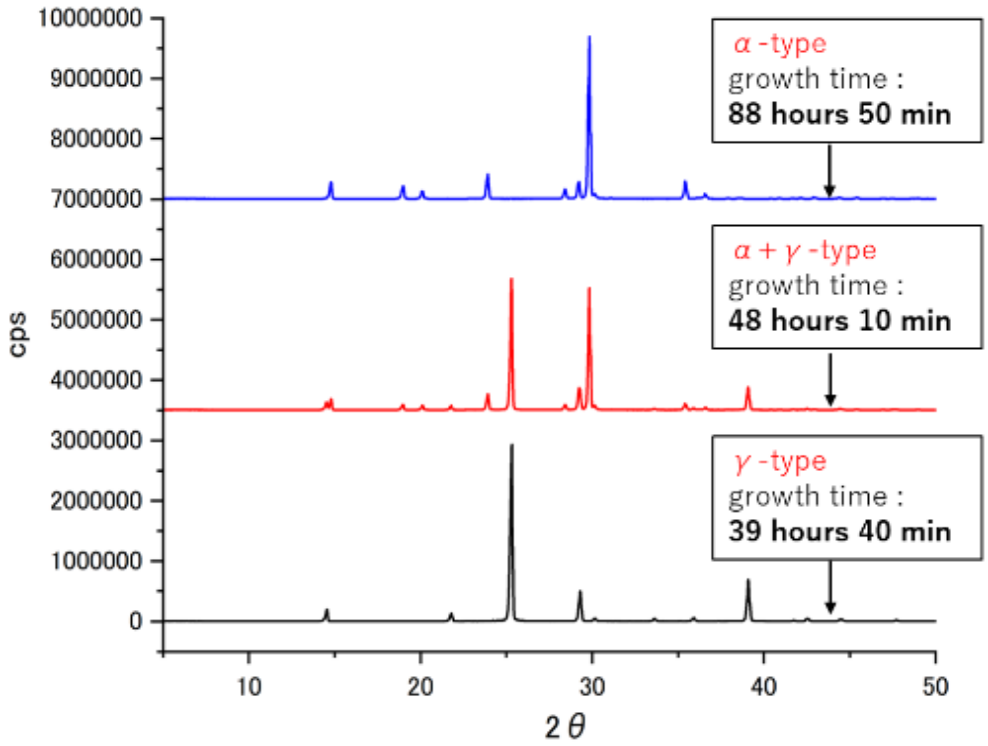



Fig.1 The X-ray patterns of glycine crystals grown in an electromagnetic irradiation at 40 GHz

# Pyroelectric effect of grown Triglycine sulfate crystals

**Kazuma Iwasaki**[1], Mana Kusama[2], Sho Fujii[3], Tsuyoshi Kimura[4], Masaya Yamamoto[5], Tadao Tanabe[6]

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Terahertz waves have the ability to penetrate plastics and are expected to be used in new plastic sorting applications. However, the development of terahertz wave detectors is currently insufficient, with only a few types available, and many of them are difficult to handle: some can be used at room temperature but have poor sensitivity, while others have high sensitivity but cannot be used at room temperature. In this study, in order to develop a highly sensitive terahertz wave detector, triglycine sulfate (TGS) crystals, which are expected to respond to terahertz waves, were prepared by a solution growth method and their response was evaluated.

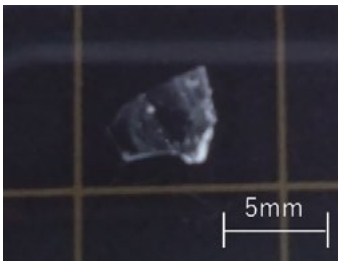


Fig.1 Crystal appearance

Figure 1 shows the appearance of the crystals used in this study. The thickness of the crystals was about 500 µm. Figure 2 shows the results of irradiating the home-made TGS crystal with a CO2 laser (ACCESS LASER, L3S-FCCL, wavelength 10.3~10.7 µm). The crystals were irradiated with the laser for 5 seconds from about 7 seconds after the start of recording. It was observed that the signal began to increase immediately after the laser oscillation, and at the point where the laser stopped, the signal increased to about 0.1 mV, and then returned to the signal value before the start of measurement after about 50 seconds. At the time of the presentation, a comparison with commercially available detectors will be made, as well as the change in response when the crystals are processed by etching or evaporation.

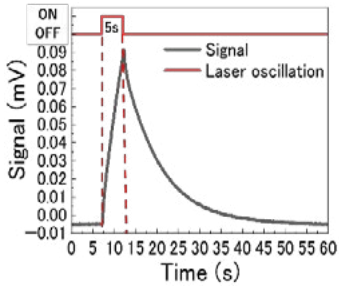


Fig.2 Response of TGS crystals fabricated by crystal growth method to a 10 µm laser wavelength

*Keywords: Terahertz wave, detector, TGS crystal, crystal growth, plastic fractionation*

# Technical **Oral Session _ Session 6**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 6 (J6)** **16:00 - 17:40, Nov. 21**

Chair : Kil-Won Moon (National Institute of Standards and Technology) 201B, 2F

16:00-16:20 **I-J1075** **[Invited] Atom Probe Study on Interface Segregation and Interphase Precipitation in Microalloyed Steels**
Hung-Wei Yen (National Taiwan University, Taiwan)

16:20-16:35 **O-J0107** **Spatial incorporation of thermal analysis with high-temperature microscope: A case study of peritectic solidification in steel**
Suk-Chun Moon (University of Wollongong, Australia)

16:35-16:50 **O-J0611** **Investigation of the Microstructure and Mechanical Properties of Steels Subjected to Laser Ablation Treatment**
Jiawei Tu (The University of Sydney, Australia)

16:50-17:05 **O-J0675** **Analysis of temperature characteristics of axle box bearings in high-speed operation of railway vehicles**
Jeongguk Kim (Korea Railroad Research Institute, Korea)

17:05-17:20 **O-J0520** **Massive interstitial solid solution medium-entropy alloys achieve ultrahigh strength and large deformability**
Chang Liu (Xi'an Jiaotong University, China)

17:20-17:40 **I-J1152** **[Invited] HAADF-STEM-EDS analysis and post APT runs for observing superfast solute transport in L12 precipitation-hardened Ni-based superalloys**
Jae Bok Seol (Gyeongsang National University, Korea)

# Atom Probe Study on Interface Segregation and Interphase Precipitation in Microalloyed Steels

**Hung-Wei (Homer) Yen[1]**, Shao-Lun Lu[1], Kou-Cheng Yang[2], Yi-Sheng Chen[1, 3, 4], Limei Yang[3, 4, 5], Julie M. Cairney[3, 4]

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## Abstract

In steels, interphase precipitation is a captivating transformation behaviour, wherein microalloy carbides nucleate at the interface during the austenite-to-ferrite transformation. Despite being the subject of study for over 50 years, the detailed mechanism underlying interphase precipitation remains unresolved. Specifically, solute partition and segregation in the vicinity of interface demand further investigation for comprehensive understanding. In this study, we employ complementary characterizations by atom probe and transmission Kikuchi diffraction, to explore the intricate relationship between interphase orientation and solute segregation in microalloyed steels. Furthermore, we utilize transmission electron microscopy to reveal the tendencies of interface precipitation concerning interphase orientation. Our findings indicate that interphase precipitation occurs through a delicate balance between interfacial mobility and solute segregation. This essential understanding is critical for controlling the occurrence of interphase precipitation at the moving interface. With these insights, we leverage this newfound knowledge to design a cold-rolled dual-phase steel strengthened by interphase-precipitated carbides. This research contributes to enabling findings from tomographic microscopy to develop advanced high-strength steels.

*Keywords: interphase precipitation; solute segregation; atom probe; transmission Kikuchi diffraction; transmission electron microscopy; microalloyed steel*

# Spatial incorporation of thermal analysis with high-temperature microscope: A case study of peritectic solidification in steel

**Suk-Chun Moon**[1], Dominic Phelan[2], Rian Dippenaar[3]

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## Abstract

High temperature confocal microscopy (HTCM) and thermal analysis techniques (e.g. differential thermal analysis (DTA) and differential scanning calorimetry (DSC)) are well-established experimental techniques. While HTCM allows for direct observation of phase transformations on the surface, events in the bulk of the material and information regarding when a phase transformation commences and finishes, cannot be explicitly measured. Thermal analysis provides data on the progress of phase transformations throughout the entirety of sample but cannot directly measure the number of nucleation events or growth kinetics at individual parent/product interfaces.

To address these issues, the authors modified an existing HTCM to incorporate thermal analysis functionality and revisited earlier studies on peritectic solidification of steel. The authors observed deep undercooling for austenite nucleation in a peritectic steel in the absence of liquid phase (i.e., without a peritectic reaction). The reasons behind this are the constrained nucleation of austenite and a limited number of nucleation sites available in the small sample that is usually used for thermal analysis. They propose that the occurrence of peritectic reaction and the degree of undercooling for austenite nucleation largely depend on the size of sample used in experiment which determines the statistical chance of delta-ferrite grain boundary multiple junctions as heterogeneous austenite nucleation sites.

This study sheds light on the challenges in studying peritectic solidification and the limitations of current experimental techniques. It emphasizes the potential of using modified HTCM that incorporates thermal analysis functionality for more accurate and comprehensive analysis of phase transformations beyond just peritectic phase transition.

*Keywords: Confocal Microscope, Thermal analysis, DTA, DSC, Peritectic Reaction*

# Investigation of the Microstructure and Mechanical Properties of Steels Subjected to Laser Ablation Treatment

**Jiawei Tu**[1], Anna Paradowska[1,2], Andrei Rode[3], Ludovic Rapp[3], Steve Madden[3], Michael Drew[2], Meera Mohan[4], Gwénaëlle Proust[1,5]

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[5] Sydney Manufacturing Hub, The University of Sydney, NSW 2006, Australia



## Abstract

Laser cleaning consists of irradiating a laser beam to targeted surfaces and is demonstrated as an effective technique for removing contaminents and paint layers from solid surfaces. It is a contact-free process that can be carefully controlled to minimise and even avoid damage to the original substrate beneath a contaminated or corroded surface. In comparison to other cleaning techniques, lasers operating in the nanosecond and femtosecond regimes offer an environmentally friendly way of cleaning structures and improves control over the surface characteristics of the underlying material. This facilitates better long-term preservation of steel structures such as the Sydney Harbour Bridge, which is the major focus of this study.

This research aims to investigate the microstructure and mechanical properties of structural steels after nanosecond laser cleaning by using various material characterisation techniques. The surface topography and microstructure of laser-ablated steels were characterised by using scanning electron microscopy (SEM) and electron backscattered diffraction (EBSD) technique. X-ray and neutron diffraction measurements were conducted to explore the near-surface and through-thickness residual stresses.

*Keywords: Material characterisation, electron backscattered diffraction (EBSD), hardness, laser ablation treatment, residual stress*

# Analysis of temperature characteristics of axle box bearings in high-speed operation of railway vehicles

**Jeongguk Kim**

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**Abstract**

Axle box bearings of high-speed railway vehicles are one of the components that make a significant contribution to ensuring the running safety of vehicles. If the axle box bearing is damaged, the temperature around the axle box rises, and if this condition persists, problems with the rotation of the axle can cause serious accidents. Therefore, temperature monitoring and management are essential for axle box bearings in high-speed railway vehicles. In this study, we would like to introduce a technology that can monitor and manage the temperature of axle box bearings. Also, we would like to introduce the manufacturing process of a module that can monitor the temperature of axle box bearings in real time by applying infrared thermography technology. As compared with the conventional method of measuring temperature using a temperature sensor, the testing results conducted in the actual field will be introduced. Temperature data measured in real situations and analysis results of temperature characteristics will also be introduced.

*Keywords: Temperature Characterization, Infrared Thermography, Axle Box Bearings, High-speed Train, Railway Vehicle*

# Massive interstitial solid solution medium-entropy alloys achieve ultrahigh strength and large deformability

**Chang Liu**

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## Abstract

Interstitial solutes, such as carbon, are effective solid solution strengthening agents. Nevertheless, when the interstitial content exceeds a critical yet low value, brittle intermetallic compounds may form, which deteriorates the homogeneous deformation ability of the alloy. Thus, the contents of interstitials in alloys are often low [1], e.g. below 3 at%. Here, through using a medium-entropy alloy as the highly distorted substitutional matrix, we have successfully solutioned massive amounts of interstitials into the alloy. We term this new class of alloys as massive interstitial solid solution (MISS) alloys [2]. For a model $(TiZrNb)_{86}O_{12}C_1N_1$ (at%) MISS alloy, the oxygen content reaches 12 at%, without forming oxides. This MISS alloy achieves an ultrahigh yield strength of 4.2 GPa, and reveals homogeneous deformation to a strain of 65% in compression at ambient temperature. Further, we used deep-sub-angstrom-resolution electron ptychography and present the first experimental evidence to directly observe individual oxygen atoms in the $(TiZrNb)_{86}O_{12}C_1N_1$ MISS alloy [3]. In addition to oxygen residing at the octahedral sites, we provide unambiguous evidence that oxygen solutes switch from octahedral to tetrahedral sites at high oxygen concentrations. This shift in position is explained by the extra cost of strain energy to accommodate interstitials when the requisite displacement of host atoms is deterred in the presence of nearby octahedral interstitials.

[1] F.C. Campbell (2008), Elements of metallurgy and engineering alloys.

[2] C. Liu *et al.*, Massive interstitial solid solution alloys achieve near-theoretical strength, *Nat. Commun.* 13 (2022) 1102.

[3] C. Liu *et al.*, Direct observation of oxygen atoms taking tetrahedral interstitial sites in medium-entropy body-centered-cubic solutions, *Adv. Mater.* (2023) 2209941.

*Keywords: Interstitials, solid solution, TEM, strength, deformability*

# HAADF-STEM-EDS analysis and post APT runs for observing superfast solute transport in $L1_2$ precipitation-hardened Ni-based superalloys

**Jae Bok Seol[1]*,** Muhammad Ishtiaq[1], Hyo Ju Bae[1], Joong Eun Jung[2], Won-Seok Ko[3], Bong-Ho Lee[4]

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**Abstract**

Here, we reported the higher yield strength in a modified IN738LC alloy than in a standard 738LC alloy at 930 ºC. Using scanning transmission electron microscopy (STEM), we revealed the presence of microtwins, and local phase transformation strengthening inside the ordered $L1_2$ phase in the deformed alloy, which sheds new light on deformation mechanisms that are not typically observed under such conditions. Our HAADF-STEM-EDS analysis and post-APT runs provided direct evidence of superfast solute transport from the FCC matrix into the ordered $L1_2$ superlattice along twin boundaries and dislocation cores. Furthermore, our STEM results provided detailed insights into the formation and distribution of microtwins, $L1_2 \rightarrow D0_{24}$ η local phase transformation along micro twin, dislocation dissociation, and superfast pipe diffusion along twin boundaries and dislocation cores at high temperatures, highlighting their potential contribution to improving the high-temperature mechanical properties of Ni-based polycrystal superalloys. Finally, we will guide new high-temperature polycrystal superalloys design.

# Technical **Oral Session _ Session 6**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 6 (K6)** **16:00 -18:10, Nov. 21**

**Chair :** Saryu Fensin (Los Alamos National Laboratory) Samda Hall B, 3F

16:00-16:20 **I-K0523** **[Invited] Development of aluminum matrix composites containing high-entropy phases**
Hyun Joo Choi (Kookmin University, Korea)

16:20-16:40 **I-K0856** **[Invited] Dislocation plasticity in a multi-principle element alloy with hexagonal closed-packed crystal structure**
Jie KUANG (Xi'an Jiaotong University, China)

16:40-16:55 **O-K0355** **Discussion on High Entropy Effect on Ligament Growth in Nanoporous TVNbMoTa Alloy**
Hidemi Kato (Insitute For Materials Research, Japan)

16:55-17:10 **O-K0059** **A new process suitable for L12-strengthened high-entropy alloys**
Jae Heung Lee (Pohang University Of Science And Technology, Korea)

17:10-17:25 **O-K0853** **Microstructure and properties of high entropy alloy fibers**
Lin Deng (University Of Science And Technology Beijing, China)

17:25-17:40 **O-K0479** **Determination of the existence composition range of CrMnFeCoNi high-entropy alloys using multiple diffusion method**
Ryuta Yurishima (Ibaraki University, Japan)

17:40-17:55 **O-K0113** **Study of the influence of alloying elements on W-containing refractory high-entropy alloy prepared by mechanical alloying**
CHUN-LIANG CHEN (National Dong Hwa University, Taiwan)

17:55-18:10 **O-K1149** **Design high entropy alloys for additive manufacturing**
Zhijun Wang (Northwestern Polytechnical University, China)

# Development of aluminum matrix composites containing high-entropy phases

Chahee Jung[1], Hansol Son[1], Jaewon Jung[2] and Hyunjoo Choi[1*]

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Aluminum matrix composites (AMCs) have been extensively studied in the future mobility industries because of their excellent mechanical properties and elastic modulus. Although carbon-based or ceramic materials have been used as reinforcement for AMCs, their poor wettability with aluminum should be overcome to develop high-strength lightweight composites.

This study employs high entropy alloys (HEAs) as reinforcement AMCs. HEAs have superior stiffness and strength as well as good good wetting ability with aluminum. Two different types of composites are suggested in this study. First, sub-micron sized HEA particles, produced by thermal plasma treatment, were dispersed in aluminum powder. The composite powder was consolidated using hot-rolling. Second, gas-atomized HEA powder and Al powder were simultaneously additive manufacturing using a multi-nozzle direct energy deposition (DED) printer. The effect of HEA phases on strengthening of Al matrix will be discussed.

# Dislocation plasticity in a multi-principle element alloy with hexagonal closed-packed crystal structure

**Jie Kuang[1],** Dongdong Zhang[2], Yuqing Zhang[3], Qinghuan Huo[4], Fuyang Tian[5], Gang Liu[6], Jinyu Zhang[7], Jun Sun[8]

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## Abstract

There is a global research surge in multi-principle element alloys (MPEAs) in recent years, but so far most studies have focused on face-center cubic (FCC) and body-center cubic (BCC) structures, largely neglecting MPEAs with hexagonal-closed packed (HCP) structures. In this work, we successfully fabricated single-phase Ti-Zr-Hf MPEAs with HCP structure (c/a ratio similar to Ti) and conducted systematic comparative studies on their dislocation plasticity and mechanical properties. Through multiscale characterization, we found that compared to pure Ti, Ti-Zr-Hf MPEAs exhibited significantly higher pyramidal slip activities. Analysis incorporating first-principle calculations revealed that this enhanced pyramidal slip activity arises not only from the conventional alloying effect, but also, interestingly, from the local fluctuations inherent to MPEAs. The modified dislocation activities are responsible for the exceptional strength-toughness combination of the present coarse-grained HCP MPEAs.

*Keywords: multi-principle element alloys; hexagonal-close packed structure; dislocation plasticity; generalized stacking fault energy; strength-toughness combination*

# Discussion on High Entropy Effect on Ligament Growth in Nanoporous TVNbMoTa Alloy

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## Abstract

Nanoporous metals have drawn considerable attention for their functional properties due to its unique 3D open cell structures. In 2011, we have introduced Liquid Metal Dealloying (LMD) method for creating porous structure in the base and half metals and alloy which are usually oxidized or etched by the conventional chemical or electrochemical dealloying methods in acid/alkali solutions as dealloying media [1]. Using LMD, nano, submicron porous Zr, V, Nb, Ta, Cr, Mo, W, Fe, C, Si and β-Ti alloy, Fe-Cr, Ni-Cr etc have been developed. Very recently, we also succeeded in preparing a nanoporous bcc-high entropy alloy (TiVNbMoTa system) with the minimum ligament/pore size~10 nm and found that its thermal ligament growth was suppressed with compared to the reported "low entropy" nanoporous metals and alloys [2]. To clarify the reasons and discuss possibility "sluggish diffusion" for high thermal stability of ligament in this nanoporous HEA, the ligament size ($d_{0.4Tm}$) prepared at the same homologous temperature (melting point normalized) and thermal activation behavior of the ligament growth in the element metal (Mo), their low and medium entropy alloys (VMo, NbMo, MoTa, VNbMo, TiVNbMo and TiVNbMoTa) are systematically investigated. The results indicated that there is a tendency that the ligament size decreased with the mixing entropy (or number of element), and especially when Ta is included. Thermal activation energy does not show the clear dependence on the mixing entropy (or number of element) of the alloys. Further investigation on TiVNbMoTa nanoporous HEA indicated that a $Ni_2Ti_1(V,Mo,Nb,Ta)_1$ ordered phase covered the dealloying front, and it disturbed the surface diffusion causing the ligament growth. In the dealloying back region, the ligament became cubic shape due to Mo-(Nb,Ta) B2 ordering. Summarizing these experimental results, the high thermal stability of the ligament size in the TiVNbMoTa HEA is caused by the ordering at the dealloying front and in the ligament itself in the dealloying back region with specific elements, rather than the "sluggish diffusion" of HEA.

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*Keywords: high entropy alloy, liquid metal dealloying, nanoporous, ligament growth, sluggish diffusion*

# A new process suitable for $L1_2$-strengthened high-entropy alloys

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## Abstract

$L1_2$ phase, with slow-growing kinetics due to its coherency with FCC phase, has gained significant attention as precipitates in high-entropy alloys (HEAs) with FCC matrix, and many alloy systems have been developed. The processing typically involves post-cold-rolling solutionizing heat treatment. However, during the solutionizing process, the accumulated dislocation density from the rolling process is completely removed, leading to a decrease in strength. On the other hand, if aging is carried out directly without solutionizing, a high proportion of high-angle grain boundaries leads to the undesired discontinuous precipitation, resulting in a significant reduction in ductility. In this study, a novel processing method utilizing hot rolling is proposed for a newly designed $L1_2$-strengthened $(FeCoNi)_{79.5-x}Cr_{10.5}Al_5Ti_5Ta_x$ (at%) high-entropy alloy. High strength and ductility are achieved simultaneously by maintaining a high dislocation density and promoting $L1_2$ phase precipitation. The strengthening mechanisms are quantified, revealing the origin of high yield strength. In this process, a refined model of precipitation strengthening mechanisms is presented compared to existing models. The alloy not only exhibits high yield strength but also shows a significant hump in the work-hardening curve, resulting in high tensile strength. This phenomenon is attributed to the rapid reduction in the average free path of dislocations due to plane slip within large grains.

*Keywords: high-entropy alloy, $L1_2$ precipitation, direct aging, strengthening mechanism, deformation mechanism*

# Microstructure and properties of high entropy alloy fibers

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## Abstract

Metallic fibers with high strength and ductility are highly desired for various engineering applications, such as pearlite steel fibers used in large cable-stayed bridges and heavy lift slings, micro fibers used in mobile phone hinges and eyeglass springs in our daily lives. However, the more complex service environment in practical applications poses significant challenges to the stability of the structure and performance of the metallic fiber. The unique design concept of high entropy alloy makes its mechanical properties have a great control range to overcoming the strength-ductility trade-off through special microstructure, which making them novel and potential candidates for high-performance fibers. This report summarizes the related research of our research group in the field of high entropy alloy fibers, including $Al_{0.3}CoCrFeNi$ millimeter-sized fibers, $AlCoCrFeNi_{2.1}$ bionic bamboo micron-sized fibers, $Al_{0.5}Cr_{0.9}FeNi_{2.5}V_{0.2}$ precipitation strengthened wires and VCoNi medium entropy alloy fibers. The research shows that the high entropy alloys with FCC structure has excellent machinability, which is conducive to obtaining smaller wire size through drawing process. Combining with the subsequent heat treatment process, the introduction of B2, $L1_2$ and κ precipitates in the FCC matrix can further improve the mechanical properties of high entropy alloy to pursued for engineering applications in a variety of extreme circumstances.

*Keywords: High entropy alloy fibers; Properties.*

# Determination of the existence composition range of CrMnFeCoNi high-entropy alloys using multiple diffusion method

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## Abstract

Exploring vast composition space with multiple elements has posed challenges in creating phase diagrams necessary for optimizing high-performance materials. To efficiently investigate phase diagrams of multicomponent systems, our group has developed a multiple diffusion method, which provides an overview of the phase diagram in a multicomponent system from a single sample. Here, we examined the phase diagram of CrMnFeCoNi alloys, an essential multicomponent system where the acquisition of a stereoscopic phase diagram is desired. The phase boundary compositions determined by the multiple diffusion method were compared with those obtained using conventional samples in equilibrium states after annealing.
By utilizing multiple diffusion samples with compositional gradients, comprehensive compositional information is obtained across vast spaces. Electron probe microanalysis facilitates the acquisition of millions of points of compositional data from sample cross-sections. Compositional data were plotted in a tetrahedral composition space, allowing the evaluation of gradients in number density defined as number of data points per volume in the composition space. Compositions exhibiting maximal gradients were regarded as boundaries of existence ranges for high-entropy phase.
Composition analysis of each phase in conventional equilibrium samples revealed that compositions of single-phase samples fall within the phase boundaries determined by the multiple diffusion method. The phase boundary compositions obtained from multiple-phase equilibrium samples are in the vicinity of them, and data from this multiple diffusion method agree with those taken by the conventional method. Thus, proper analysis of composition mapping data from multiple diffusion samples provides continuous and comprehensive phase boundaries in phase diagrams for multicomponent systems.

*Keywords: Multi-component systems, Multiple diffusion, Combinatorial, High-entropy alloys.*

# Study of the influence of alloying elements on W-containing refractory high-entropy alloy prepared by mechanical alloying

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**Abstract**

Refractory high-entropy alloys (RHEAs) are important candidate materials for the design of structural materials in advanced nuclear energy systems. In this study, W-containing RHEAs were fabricated by mechanical alloying. The effects of different alloying elements, phase formation, sintering temperatures, and mechanical alloying on microstructural evolution and mechanical properties of the WMoVTiCr, WVTaTi, and WVTaTiCr model alloys were investigated. The results show that the model alloys mainly consist of BCC solid solution phase. Ti and Ta elements can significantly affect the formation of complex oxide particles. The presence of Cr promotes the formation of the (Cr, Ta)-Laves phase. The dispersed oxide particles and the second phases play an important role in determining the microstructure development, sintering behaviour, and mechanical properties of the model alloys.

*Keywords: mechanical alloying, refractory high entropy alloy, sintering, the second phase*

# Design high entropy alloys for additive manufacturing

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**Abstract**

High entropy alloys (HEAs) with multi-principal elements provide opportunities for additive manufacturing of high-performance metallic materials. The development of HEAs significantly widens the alloy design space, which is conducive to obtaining more advanced metallic structural materials with unique phase compositions, stacking-fault energies, and associated deformation mechanisms. During the past decade, we focus on the fundamental physical metallurgy of HEAs by considering the solid solution solubility, phase selection and strengthening mechanism. These preliminary investigations pave the way for additive manufacturing. We have explored several HEAs for additive manufacturing, the single solid solution alloys, precipitation hardening alloys and eutectic alloys. All the designed alloys show well printability and good mechanical properties.

Topic area: High-Entropy Materials and Amorphous Materials (K)

*Keywords: high-entropy alloys, additive manufacturing*

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# Technical **Oral Session _ Session 6**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 6 (L6)** **16:00 -17:55, Nov. 21**

Chair : Caroline Sunyong Lee (Hanyang University), Yoshimi Watanabe (Nagoya Institute of Technology) 202B, 2F

16:00-16:30 **K-L1040** **[Keynote] Nanofibre Membranes for Energy Harvesting -Applications in Triboelectric Nanogenerators**
Jin Zhang (University of New South Wales, Australia)

16:30-16:50 **I-L1094** **[Invited] A study on the development of multi-component alloys for the nanocomposite coatings and their properties**
Kyoung Il Moon (Korea Institute of Industrial Technology, Korea)

16:50-17:10 **K-L1156** **[Keynote] Multifunctional Nanoparticle Sensor Fabricated by Solvent-free Aerodynamically Focused Nanoparticle Printing**
Sung-Hoon Ahn (Seoul National University, Korea)

17:10-17:25 **O-L0063** **Effect of granule shape parameters on the melting behaviors of mold powder**
Fuhang Chen (Chongqing University, China)

17:25-17:40 **O-L0089** **Shear deformation behavior of heterostructured materials**
GangHee Gu (Pohang University of Science and Technology, Korea)

17:40-17:55 **O-L0132** **Microstructural Evolution and Annealing Behavior of Cr-Coated Zry4 Prepared by Pulsed Laser Deposition**
Bo LI (The University of Tokyo, Japan)

# Nanofibre Membranes for Energy Harvesting -Applications in Triboelectric Nanogenerators

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## Abstract

Nanofibre membranes have been used in preparing next generation of flexible energy harvesting devices and self-powered sensors, e.g., triboelectric nanogenerators (TENGs). This work studies the hybridization effect of silver nanowires (AgNWs) and perovskite oxide nanocrystals on the properties and performance of TENGs constructed from electrospun composite nanofibre layer. Mn-doped $(Bi0.5Na0.5)TiO_3$-$BaTiO_3$ (Mn-BNT-BT) nanocrystals were used as semi-conductive perovskite oxide fillers and AgNWs were used as conductive fillers for the study. Poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) fibre mat with embedded hybrid fillers was electrospun into composite fibre mats and applied as the tribo-negative layer. With 5% AgNWs and 5% of Mn-BNT-BT nanocrystals, a high peak open-circuit voltage of 2170 V and a high power density of 47 $W/m^2$ was achieved by the TENG, which significantly exceeded the output values of the current PVDF-based TENGs. Schottky junctions were formed through direct contacts between the conductive silver nanofillers and semi-conductive perovskite oxide nanofillers, which facilitated with the charge movement from AgNWs to PVDF-HFP and reduced electron dissipation. These high performance TENGs have great potential to be utilized to harness biomechanical energy for sustainable power supply for electronic devices.

*Keywords: Energy Harvesting, Nanofibres, Electrical Output, Triboelectric, Sustainable*

# A study on the development of multi-component alloys for the nanocomposite coatings and their properties

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**Abstract**

While modern industries are becoming more sophisticated, diversified, and globalized, they requires the development of smart materials have multi-functionality, high mechanical properties, and extreme durability. Also they could be prepared environmentally friendly and energy efficiently. At the same point of view, the smart coating materials capable of simultaneously expressing various mechanical properties or opposite properties such as high hardness with high toughness, high electricity with high corrosion resistance are attracting attentions as an versatile and useful materials in the future. In particular, there is an urgent needs to develop a novel coating materials capable of stably maintaining microstructures and mechanical properties in various external environments, unlike conventional coating materials whose properties and structures are easily changed by the some harsh environments. To get this kinds of objects, the coating material with multi-components are essential. But if the materials should be prepared with one phase with multi components, they could have only one properties. So, nanocomposites with various phases to realize the various properties should be formed. So, it is necessary to develop a coating layer composed of various components those could be formed various phases and more complex structures.

In this study, various single alloy materials with various compositions such as Mo-Cu-X and Zr-Cu-X, and Ti-Al-X have been tried to be prepared by powder metallurgy methods such as atomization, mechanical alloying, and Spark Plasma Sintering (SPS). The properties of as-prepared nanocomposite coatings will be summarized in this present.

*Keywords: Nanocomposite coating, Alloying Targets, Opposite Properties, Various Applications, Surface Engineering*

# Multifunctional Nanoparticle Sensor Fabricated by Solvent-free Aerodynamically Focused Nanoparticle Printing

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## Abstract

A real-time, accurate monitoring process is a basic and crucial enabler of smart manufacturing operations, digital twin applications, and structural health monitoring systems. Vibration sensors, strain sensors, and temperature sensors play major roles in the measurement and monitoring of industrial devices, architectures, and movables. However, vibration and strain sensors with high sensitivity and large stretchability at once remain as technological limitations. To overcome these limitations, we fabricated an interoperable silver nanoparticle sensor using a solvent-free aerodynamically focused nanomaterials (AFN) printing system. This AFN printing system is a direct printing technique for stretchable and conductive pattern printing onto a flexible substrate at room-temperature and low vacuum conditions. Since it does not require any post-process and after-treatment, highly sensitive sensors can be fabricated at a cost of several cents each. Microscale porous properties of AFN printed pattern enabled sensors to perform high sensitivity and large stretchability. Using a fabricated AFN sensor, we evaluated the sensing performance and demonstrated the measurement independence of vibration, strain, and temperature sensing. Furthermore, vibration, strain, and temperature were each measured separately in real-time by using the proposed signal separation algorithm based on the Kalman filter, Fourier, and ensemble learning. Finally, we applied the printed nanoparticle sensor to drone condition monitoring to predict the motion of a drone.

*Keywords: Nanoparticle sensor, Multifunctional sensor, Strain sensor, Vibration sensor, Highly sensitive*

# Effect of granule shape parameters on the melting behaviors of mold powder

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## Abstract

Hollow particle mold powder is an essential functional material in the continuous casting process, and its melting behavior significantly influences continuous casting. The existing research mainly focuses on the influence of carbonaceous materials and carbonate on the melting behavior of mold powder. The influence of the shape parameters of powder particles needs to be clarified. In this study, the influence of the shape parameters of the powder particles on the melting behavior is investigated using the melting rate test method based on a copper bath. The results show that the smaller the particle size of the powder, the worse the permeability of the powder layer and the better the thermal insulation, which is beneficial to the melting of the mold powder. When the sphericity of the mold powder particles is poor and the porosity is large, uneven sintering is prone to occur during the heating process, causing agglomeration shrinkage, resulting in uneven pores in the sintered layer, which affects the melting uniformity of the mold powder.

*Keywords: continuous casting, mold powder, melting behavior, shape parameters*

# Shear deformation behavior of heterostructured materials

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**Abstract**

Metallic materials with heterogeneous microstructure are attracting great attention as next-generation structural materials primarily attributed to their excellent strength-ductility combination in tensile properties. Heterogeneous interfaces between dissimilar domains lead to additional enhancement of tensile properties by accumulating geometrically necessary dislocations near the interfaces during tensile deformation. However, the deformations that structural materials subject to include not only tensile deformation mode, but also shear, torsion, and bending deformation modes. It is therefore necessary to verify whether a heterogeneous strengthening effect is possible in various deformation modes as well as in tension to use heterostructured materials as structural materials. For the first time, this study investigated the effect of heterogeneous microstructure on shear deformation behavior. It was verified through experiments and finite element simulations using Al1050/low-carbon steel/Al1050 clad metal sheets with sharp heterogeneous interfaces.

*Keywords: Shear deformation, Heterostructured material, Clad metal, Geometrically necessary dislocation, Finite element method*

*Topic area: Composite, Coating and Hetero-Materials*

# Microstructural Evolution and Annealing Behavior of Cr-Coated Zry4 Prepared by Pulsed Laser Deposition

**BO LI[1],** Huilong Yang[3], Reuben Holmes[1], Lijuan Cui[2], Sho Kano[2], Hiroaki Abe[1,2]

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**Abstract**

The development of accident-tolerant fuel (ATF) is crucial for improving the safety and efficiency of nuclear power plants. In this study, a Cr-coating layer with a uniform thickness and void-free interface was successfully prepared onto Zry4 using pulsed laser deposition (PLD), with the aim of exploring its potential application in ATF.

The microstructural stability of the Cr-coating layer was investigated through ex-situ and in-situ annealing combined with grazing incidence X-ray diffraction (GIXRD) analysis and transmission electron microscopy (TEM) observation. The microstructure of the Cr-coating layer consisted of two distinct layers: a nanocrystalline layer in contact with Zry4 with small grain size and no fixed shape, and a columnar crystal layer.

During ex-situ and in-situ annealing, recrystallization and grain coalescence were observed at temperatures of 300-400°C and >400°C, respectively, which led to an intensified (110)-texture due to its high reticular density and low energy close-packed. The in-situ heating experiments also revealed the formation of Kirkendall cavities in the thin film specimens, which were not observed in the block specimens in the ex-situ experiments, due to size effects.

Overall, the results of this study provide valuable insights into the microstructural stability of Cr-coated Zircaloy ATF under elevated temperatures, which is essential for its potential application in nuclear engineering. The successful preparation of a Cr-coating layer with a uniform thickness and void-free interface using PLD offers a practical method for the development of ATF, and further research is needed to optimize its microstructural stability and performance under various conditions.

*Keywords: Accident tolerant fuel, Cr coating, interface, microstructure, PLD.*

# Technical **Oral Session _ Session 6**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 6 (M6)** **16:00 -17:50, Nov. 21**

**Chair :** Dmitry Golberg (Queensland University of Technology), Dongyun Lee (Pusan National University) **402, 4F**

16:30-16:50 **I-M1151** **[Invited] Hydrogen effects on the nanomechanical behavior of nanostructured high-entropy alloys**
Yakai Zhao (Agency For Science, Technology And Research (A*STAR), Singapore)

16:50-17:05 **O-M0348** **Effect of layer thickness on the fatigue properties of accumulative roll bonded Cu/Nb laminates**
Koki Yasuda (The University of Tokyo, Japan)

17:05-17:20 **O-M0823** **Grain Boundary Distributions of Extra-Hardened Al-3mass%Mg alloy by ECAE**
Taiki Morishige (Kansai University, Japan)

17:20-17:35 **O-M0825** **Mechanical Characterization of Thin Films via Constant Strain Rate Membrane Deflection Experiments**
Gi-Dong Sim (Korea Advanced Institute of Science and Technology, Korea)

17:35-17:50 **O-M0964** **High-throughput bulk nanostructured metal and alloys fabrication via ultrasonic shot peening and electrical pulsing treatment**
Fei Yin (Wuhan University of Technology, China)

# Hydrogen effects on the nanomechanical behavior of nanostructured high-entropy alloys

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## Abstract

Grain boundary acts as an important role in affecting the hydrogen embrittlement behavior in alloys. By recourse to nanomechanical testing and analysis, the hydrogen effects in both single- and dual-phase high-entropy alloys (HEAs) processed by high-pressure torsion can be readily understood, of which mechanical testing is otherwise difficult due to the relatively small sample size. For single-phase face-centered cubic (FCC) CoCrFeNi and CoCrFeMnNi, the marked change in grain size from coarse-grained to nanocrystalline can affect the hydrogen absorption and plastic deformation behavior. Thermal desorption analysis of the hydrogen-charged samples proved that grain boundaries act as hydrogen traps and thus largely increase the hydrogen contents in the nanocrystalline samples. A direct comparison in the hydrogen absorption between two HEAs confirms that both chemical composition and grain size are crucial factors contributing to the hydrogen solubility of the HEAs. For dual-phase $Al_{0.7}$CoCrFeNi HEAs containing both FCC and body-centered cubic (BCC) phases, the influences of hydrogen on the thermal desorption and nanoindentation responses of nanocrystalline HEA were compared with the coarse-grained alloy. The plastic zone size and indentation size effects were carefully considered to identify the distinct contributions of the constituent phases to the hardness and its variation with hydrogen charging. Results show that the FCC phase is susceptible to a higher degree of hydrogen-induced hardening than the BCC phase.

*Keywords: High-entropy alloys; nanoindentation; hydrogen effects; nanocrystalline; high-pressure torsion.*

# Effect of layer thickness on the fatigue properties of accumulative roll bonded Cu/Nb laminates

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## Abstract

Cu/Nb metallic laminates, produced by accumulative roll bonding (ARB), have attracted attention as a structural material that combines high strength and electrical conductivity, and the effects of dissimilar interfaces on their tensile properties and fracture behavior have been reported. However, the fatigue properties of Cu/Nb laminates have not been clarified in detail. In this study, four-point bending fatigue tests were performed on Cu/Nb laminates to evaluate the fatigue properties.

The fatigue behavior was analyzed by surface observation using optical microscope during the test and by scanning electron microscopy (SEM) after the test. Four-point bending fatigue tests were performed at a stress ratio of 0.1 and a frequency of 20 Hz, with varying stress amplitudes. The specimen thickness was 1 mm, width was 5 mm, and the longitudinal direction was adjusted to be rolling direction (RD) or transverse direction (TD). The cracks were observed by SEM on the side surface parallel to RD and normal direction (ND). The cracks propagated diagonally and branched out near the thick Nb phase. The branching cracks were observed to propagate along the phase interfaces. The effects of anisotropy, interfaces between different phases, and layer thicknesses on fatigue properties were discussed. It was shown that the number of cycles to failure of the RD specimens was larger than that of the TD specimens.

*Keywords: Cu/Nb laminated, fatigue properties, four-point bending fatigue tests, interfaces, anisotropy.*

# Grain Boundary Distributions of Extra-Hardened Al-3mass%Mg alloy by ECAE

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## Abstract

Severe plastic deformation is an effective technique for obtaining ultrafine-grained aluminum alloy. SPD-ed Al alloy has high dislocation density and thus the strength exceeds the estimated it by the grain size using Hall-Petch relationship. This higher dislocation density originates from the microstructural evolution during dynamic recrystallization. The excess strain during SPD processing was introduced and was remained in DRX grains. SPD processed Al-Mg alloy represents especially large dislocation strengthening not only grain refinement strengthening. This is because Al-Mg alloy has low stacking fault energy (SFE). The dislocation rearrangement is suppressed during DRX in low SFE alloys. As a result, the microstructure is extremely fine-grained with high dislocation density in grain interior. Therefore, the grain boundary of the SPD processed Al-Mg alloy has a variety of the distributions. For example, low angle grain boundary frequently distributes in low-strained specimen because the dislocation introduction and rearrangement are not sufficiently during SPD. On the other hand, fully DRX-ed specimen has large amount of high angle grain boundary. The grain boundary distributions are variable by degree of processing and subsequent annealing. In this study, the effect of grain boundary distributions such as the fraction of low angle grain boundary and dislocation boundary (sub-grain boundary) on the strengthening of Al-3 mass%Mg alloy was investigated.

*Keywords: Severe plastic deformation, ultrafine-grained materials, aluminum alloy, equal channel angular extrusion, low angle grain boundary*

# Mechanical Characterization of Thin Films via Constant Strain Rate Membrane Deflection Experiments

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## Abstract

Thin films are widely used as functional and structural elements in micro-electronic devices, large-scale integrated circuits, thin-film solar cells, electrical sensors, and electronic textiles. Understanding the mechanical behavior of thin films at different length scales and environmental conditions is essential for the design of reliable devices. However, it is difficult to precisely measure the properties of small-scale materials with the methods that are employed for bulk materials; probing micro/nano scale samples is challenged by the inherent difficulties associated with fabricating and handling of extremely small specimens.

In this presentation, I will introduce experimental studies utilizing micro/nano-scale manufacturing and mechanical characterization techniques to understand the mechanical behavior of small-scale materials. Specifically, our recent development of a constant strain rate membrane deflection experiment (MDE) technique that enables high-throughput measurement of in-plane mechanical properties of metal thin films will be introduced. The mechanical behavior of freestanding metal thin films (gold, aluminum, and nickel-molybdenum-tungsten alloy) is characterized using micro-tensile testing and MDE. Micro-tensile and membrane samples are simultaneously fabricated on a single wafer to avoid microstructural differences. By comparing with micro-tensile tests, it is demonstrated that the stress-strain curve of freestanding metal thin films can be successfully measured via constant strain rate MDE. I will also demonstrate that this technique can be utilized for accelerated exploration of the chemical composition effect on the mechanical behavior of advanced structural materials such as shape memory alloys.

*Keywords: Membrane deflection experiment, Micro-tensile testing, Mechanical properties, Metal thin film, Constant strain rate*

| O-M0964 |

# High-throughput bulk nanostructured metal and alloys fabrication via ultrasonic shot peening and electrical pulsing treatment

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## Abstract

Nanostructured metal and alloys are a class of emerging materials due to its extraordinary mechanical, chemical and biological properties. In this talk, we will present our recent research work on an efficient high-throughput bulk nanostructured metal and alloys fabrication method namely, ultrasonic shot peening (USP) plus electrical pulsing post-treatment. The basic theory, mathematical modelling and dynamic analysis of the USP process will be demonstrated and an ultrastrong ductile and stable nanocrystalline steel with intermetallic nanoparticles uniformly dispersed at nanoscale fabricated via USP will be highlighted. Additionally, the effect of the electrical pulsing treatment (EPT) process on the microstructure of the as-USPed metal and alloys will be demonstrated. Finally, the potential applications of the USP plus EPT for mechanical enhancement of the engineering components will be discussed and proposed.

**Keywords:** Gradient nanostructure, Severe plastic deformation, Ultrasonic shot peening, Electrical pulsing treatment, Engineering materials.

# Technical **Oral Session _ Session 6**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 6 (N6)** **16:00 - 17:40, Nov. 21**

**Chair :** Gang Li (Deakin University), Yong Joo Kim (Kookmin University) 203, 2F

16:00-16:30 **K-N1031** **[Keynote] Generative AI to Accelerate Discovery of Materials**
Truyen Tran (Deakin University, Australia)

16:30-16:50 **I-N0544** **[Invited] High-Throughput Computational Screening and Machine Learning Modeling of Janus 2D III-VI van der Waals Heterostructures for Solar Energy Applications**
Baisheng Sa (Fuzhou University, China)

16:50-17:10 **I-N** **[Invited]**
Tiff Walsh (Deakin University, Australia)

17:10-17:25 **O-N0369** **Effects of point defects on hydrogen diffusivity in B2-type PdCu alloys: A kinetic Monte Carlo study**
Akihiro Mitsuhara (Nagoya University, Japan)

17:25-17:40 **O-N1015** **Electrochemical stability map of bimetallic nanoparticles**
Hongryol Jeon (Korean Institute of Science And Technology, Korea)

# Generative AI to Accelerate Discovery of Materials

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## Abstract

Generative AI represents a pivotal moment in computing history, opening up new opportunities for scientific discoveries. By harnessing extensive and diverse datasets, we can construct new general-purpose Foundation Models that can be fine-tuned for specific prediction and exploration tasks. This talk introduces our research program, which focuses on leveraging the power of Generative AI for materials discovery. Generative AI facilitates rapid exploration of vast materials design spaces, enabling the identification of new compounds and combinations. However, this field also presents significant challenges, such as effectively representing crystals in a compact manner and striking the right balance between utilizing known structural regions and venturing into unexplored territories. Our research delves into the development of a new kind of generative models specifically designed to search for diverse molecular/crystal regions that yield high returns, as defined by domain experts. In addition, our toolset includes Large Language Models that have been fine-tuned using materials literature and scientific knowledge. These models possess the ability to comprehend extensive volumes of materials literature, encompassing molecular string representations, mathematical equations in LaTeX, and codebases. We explore the open challenges, including effectively representing deep domain knowledge and implementing efficient querying techniques to address materials discovery problems.

*Keywords: Generative AI, materials discovery, crystals modelling, Large Language Models, Foundation Models.*

# High-Throughput Computational Screening and Machine Learning Modeling of Janus 2D III-VI van der Waals Heterostructures for Solar Energy Applications

**Baisheng Sa**[1], Zhimei Sun[2]

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## Abstract

Two dimensional Janus III-VI monolayers and corresponding van der Waals (vdW) heterostructures present immense application potential in the solar energy conversion areas. By combing high-throughput density functional theory calculations and machine learning methodology, the establishing and understanding of a complete database for the 2D Janus III-VI vdW heterostructures is of great interest and importance for their further applications in solar energy related areas.

In this talk, we will present our recent work on the materials screening and machine learning modeling to accelerate the discovery of promising photocatalytic and photovoltaic candidates in Janus III-VI vdW heterostructures. A comprehensive database for totally 19926 heterostructures has been proposed according to the high-throughput first-principles calculations. It is highlighted that we develop an accurate machine learning model using only atoms and bonds as descriptors based on the crystal graph convolutional neural network framework. Besides, 1035 Janus III-VI vdW heterostructures have been screened out according to the essential criteria of stability. Moreover, we find 66 and 71 potential candidates for photocatalysis and solar cell from further application driven screening. Interestingly, the screened type-II SeInAlS/SeGaAlTe heterostructure with a band gap of 1.18 eV is highlighted as an internal electric field driven asymmetrical photocatalyst. On the other hand, the type-II $Al_2STe/Al_2SSe$ heterostructure solar cell presents high power conversion efficiencies higher than 21 % both from the microscopic and mesoscopic views.

*Keywords: High-throughput density functional theory calculations; materials database; graph convolutional neural network; Janus III-VI monolayers; solar energy applications.*

| O-N0369 |

# Effects of point defects on hydrogen diffusivity in B2-type PdCu alloys: A kinetic Monte Carlo study

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## Abstract

Hydrogen permeable alloys have attracted attention because they can purify hydrogen gas to an ultrahigh level in a single process. A Pd-53mol%Cu alloy with the B2 structure is one of the practical Pd-based membranes for hydrogen purification. However, the hydrogen permeability of the Pd-53mol%Cu alloy decreases significantly at below 473 K because of the reduction in hydrogen diffusivity in the alloy. It has also been reported that the antisite Cu atoms in the alloy inhibit hydrogen diffusion and the Cu vacancies strongly trap hydrogen atoms [1,2]. It is important to elucidate the quantitative effects of these point defects on hydrogen diffusivity in B2-type PdCu alloys in order to apply the alloy to hydrogen purifications at low temperatures.

In this study, we developed a numerical framework for the quantitative evaluation of hydrogen diffusivity in the presence of antisite Cu atoms or Cu vacancies, based on kinetic Monte Carlo (kMC) method. The effects of these point defects on the hydrogen diffusivity of B2-type PdCu were investigated by calculating the hydrogen diffusion coefficients as a function of temperature, hydrogen concentration, and point defect concentration.

The results show that the effects of antisite Cu atoms does not significantly inhibit hydrogen diffusion, while the presence of Cu vacancies markedly reduces the hydrogen diffusivity. The predicted hydrogen diffusivity agreed well with the experimental data. These results suggest that Cu vacancies are the dominant factor in the decrease in hydrogen diffusivity at low temperatures.

[1] A. Mitsuhara et al., Collected Abstracts of the 2022 Autumn Meeting of the Japan Inst. Metals 2022 No. 168.
[2] A. Mitsuhara et al., *J. Jpn. Inst. Met.* **86** 140–148 (2022).

*Keywords: Hydrogen diffusion, Hydrogen permeation, Kinetic Monte Carlo method.*

# Electrochemical stability map of bimetallic nanoparticles

**Hongryol Jeon[1],** Kihoon Bang[2], Sangsoo Han[3] (centered, 12-point Times New Roman, presenting author's name is bolded and underlined)

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## Abstract

Bimetallic nanoparticles have received substantial attention in the past decades for their applications in numerous areas, including catalysis and energy. Especially, Pt-Co alloy catalysts have been developed to reduce the high material cost of Pt and enhance oxygen reduction activity. One of the most challenging issues is how to empower the nanocatalysts electrochemical stability for a wide commercialization of PEMFC. Experimentally observed degradation mechanisms of real-size alloy nanoparticles such as dissolution, and adsorbate-induced segregation are not well explained by current quantum simulation methods due to high computational costs. Here, we demonstrate a methodology predicting the electrochemical degradation behavior of real-size alloy NPs under different electrochemical environments. By using multi-scale simulation and our machine learning model, we can accurately predict the adsorption energy of not only pure NPs but also bimetallic alloy NPs with different size and compositions. By using monte carlo simulation, we can predict the chemical ordering of real-size alloy NPs. Our modified BE-CGCNN machine-learning model is superior to others because it can reflect the effect of size, morphology, composition, and adsorbate coverage on adsorption energies. After accurately predicting adsorption energies, we can build a reliable surface pourbaix diagram of alloy NPs. This surface pourbaix diagram can be further applied to explain electrochemical degradation behavior such as adsorbate-induced segregation, dissolution which can be observed experimentally in real-size alloy nanoparticles. This scheme can be applied to other alloy NPs, which provides a fast and general framework for the assessment of electrochemical stability of alloy NPs.

*Keywords: Surface Pourbaix diagram, BE-CGCNN, chemical ordering, oxidation, adsorbate-induced segregation*

# Technical **Oral Session _ Session 6**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 6 (O6)** 16:00 -17:45, Nov. 21

Chair : Kyoung-Tae Park ( Korea Institute Of Industrial Technology), Taichi Murakami (Tohoku University) 401, 4F

16:00-16:20 **I-O0739** **[Invited] Trends of rare earths recycling and materialization for a circular economy**
Taek-soo Kim (Korea Institute of Industrial Technology, Korea)

16:20-16:40 **I-O0308** **[Invited] New Carbon Recycling Ironmaking Process using Carbon-Iron Ore Composite**
Taichi Murakami (Tohoku University, Japan)

16:40-17:00 **I-O0413** **[Invited] Challenges and Potential Solutions for Steel Recycling with Tramp Element**
Ichiro Daigo (The University of Tokyo, Japan)

17:00-17:15 **O-O0638** **Production of High purity rare metals by Electron Beam Melting**
Kyoung-Tae Park (Korea Institute of Industrial Technology, Korea)

17:15-17:30 **O-O0618** **Extraction of neodymium halide from NdFeB scrap**
Jaeyeol Yang (Korea Institute of Industrial Technology, Korea)

17:30-17:45 **O-O0793** **Pyrometallurgical processing of industrial wastes for recovery of precious metals**
HyunJu Kim (Hanyang University, Korea)

# Trends of rare earths recycling and materialization for a circular economy

**Taek-Soo Kim[1,2]**

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## Abstract

Rare Earth (RE) based magnets are indispensable for these technologies, and Korea is totally depending on import for compounds or composites of REs as the country lacks in natural resources. Effect on rare earth supply chain significantly affects Korea's transition towards a green economy. However, rare earth ores with industrial value are distributed in only a few countries, and China accounts for over 87% of the total rare earth production due to environmental pollution generated in the process of producing rare earth metals. As a result, securing stable sources of rare earths has become increasingly important.

The recycling of rare earth permanent magnet can be promised alternatives to become stable of supply risk of rare earth elements. with the emergence of eco-friendly policies, rare earth elements in permanent magnets used in electric vehicle drive motors are emerging as the largest demand source. The rare earth permanent magnet is the application field where rare earth is used the most, and the standard composition contains about 25% of Nd, which are the main components, and about 0~10% of Dy. In this work, to secure competitiveness in China's high-tech industries surrounding rare earth resources, we discuss that it is essential to review the trends in major countries, discuss the problems and prospects for resource phenomena, and secure stable sources of demand industries.

*Keywords: Rare Earth Magnets, Rare earth elements, Recycling, Liquid Metal Extraction, circular economy*

# New Carbon Recycling Ironmaking Process using Carbon-Iron Ore Composite

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## Abstract

Carbon neutrality of the society is the worldwide issues. Especially, iron- and steel industry consumes a huge amount of fossil fuel because approximately 2 billion tons of steel produces in the world. Therefore, many studies have been developed such as hydrogen reduction and carbon recycling processes. Reduction of iron ore by hydrogen generates not carbon dioxide but water vapor. It leads to drastically decrease in carbon dioxide emission. However, the refining process of molten steel using converter is required to use carbon oxidation reaction while there is no carbon in the hydrogen reduction process. On the other hand, the previous carbon recycling process is that carbon monoxide produces from carbon dioxide which is obtained by the separation from the exhaust gas from blast furnace. The reduced iron can be produced by carbon monoxide, but it is very difficult to produce molten pig iron which is useful for the refining process. To produce molten pig iron, new carbon recycling ironmaking process was suggested. This process is consisted of carbon recycling system by carbon deposition using porous iron whisker and production of molten pig iron using recovered carbon-iron ore composite. The recovered carbon is composed of solid carbon and cementite. Using this recovered carbon, the composite reduced at lower temperature than that using conventional carbonaceous materials. By heating up to 1573 K, the molten pig iron nuggets were obtained on the surface of the composite sample.

*Keywords: Carbon neutrality, Reduction of ore, Carburization, Carbon-iron ore composite, Porous iron*

# Challenges and Potential Solutions for Steel Recycling with Tramp Element

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**Abstract**

The higher content of tramp elements is a concern in steel recycling. Contamination paths of tramp elements are foreign materials mixed in steel scrap due to insufficient separation and alloying elements in and plating elements on different types of steel. Therefore, tramp element contents in steel scrap cannot be identified before melting. This concern may lead to two new directions: technological developments in materials engineering in which a certain amount of tramp elements is a prerequisite and in composition analysis on scrap without melting. For the first direction, very limited information is available on the possible impurity contents in recycled steel. Therefore, the content of impurity elements in recycled steel was determined via elemental analysis of randomly sampled steel bars. Of the twenty-three impurity elements considered, fifteen elements were found to be mixed in the recycled steel. The average and distributions of fifteen impurity element contents in Japan are quantified. Quite a large variance of the impurity contents would be a problem when those scraps are consumed for high-function steel. For the second direction, a large quantity of transactions, various shapes of pieces of steel scrap, heavier weight of each piece of steel scrap, and heterogenous distribution of foreign materials are reasons which make it difficult to quantify impurity contents in steel scrap. Here, one of the promising measures is deep learning approaches for image analysis which have been dramatically developed recently. Image analysis techniques for the image of steel scrap, which has different characteristics from other objects, are under development.

*Keywords tramp elements, steel recycling, composition analysis, average impurity ccontents, image analysis.*

# Production of High purity rare metals by Electron Beam Melting

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## Abstract

This study investigated the process of producing ingots from rare metals with high melting points, including molybdenum, tantalum, and tungsten, using the electron beam melting method. Ingots produced through melting and casting processes are widely used in various industrial fields, such as semiconductors and refractory materials. To produce ingots with high purity, it is crucial to establish the optimal conditions for volatilizing impurities remaining in the material. As this process involves applying energy of several thousand degrees, we employed finite element analysis to predict the electron beam output required for homogeneous ingot production. This enabled us to understand the temperature distribution of the material and the defect state inside the ingot according to the electron beam output. In addition, we conducted thermodynamic calculations to confirm the volatilization behavior of impurities for predicting the amount of impurity removal inside the produced ingots. This led to minimizing the defects inside the ingot and producing ingots with high purity. The results of this study can contribute to the improvement and efficiency of the process of producing high-purity rare metal ingots using electron beam melting.

*Keywords: Electron beam melting, Rare metals, Continuous casting process, removal impurities process, Ingot*

# Extraction of neodymium halide from NdFeB scrap

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**Abstract**

In this study, the magnesium halide exchange reaction was performed between NdFeB and ternalry chloride salt or fluoride salt. The halide reaction between NdFeB strap and Mg halides were carried out at 873 K(chloride salt) and 1,073 K(fluoride salt) in an argon ambience, respectively. After the reaction, the Nd halides were separated from the residual salt. At this time, it was confirmed using XRD that the Nd halide samples extracted in the form of NdF or NdCl. Then the extraction rate of Nd was evaluated. As a results, the sample was extracted the extraction rate of Nd were 84.59% using chloride salt and 98.64% using fluoride salt. It was confirmed that fluoride salt is more effective at extracting Nd than chloride salt due to the dispropornation.

*Keywords: Rare Earth, NdFeB Magnet, Extraction, Magnesium Halide, Recycling*

# Pyrometallurgical processing of industrial wastes for recovery of precious metals

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## Abstract

With rapid technological innovations and market expansion, the amount of electronic waste and spent catalyst increases rapidly in the past decades. Electronic waste and spent catalyst contain large amounts of precious metals (e.g. Ag, Au and Pd). Therefore, such wastes may be considered as a secondary source of valuable metals. Due to the conflicts of limited natural resources and increasing demands, as well as their economic value, it is essential to recycle precious metals from secondary resources.

This study aims to recover precious metals from petrochemical waste catalysts and copper sludge containing precious metals such as silver, palladium, etc. through the pyrometallurgical smelting process. When mixing a petrochemical waste catalyst consisted of $Al_2O_3$ and copper sludge, the content of $Al_2O_3$ was limited to less than 30 wt%, i.e., catalyst ratio was varied from 10 to 30%, and the expected slag was the $CaO$-$Cu_2O$-$Al_2O_3$-$Fe_2O_3$-$SnO_2$-$SiO_2$ system. The smelting reduction experiment was conducted at 1500℃ in an Ar atmosphere using a high frequency induction furnace. At this time, the solid carbon contained in the copper sludge served as a reducing agent.

As a result of the experiment, due to palladium and silver have high solubility in liquid copper, they are collected in copper alloy. The recovery rate of precious metals in copper alloy decreases as catalyst ratio increases. Slag with a high $Al_2O_3$ content has the lowest terminal velocity due to its high viscosity. Therefore, Copper particles, including valuable metals, are heavily present in the slag. So, slag viscosity and terminal velocity of copper particles need to be precisely controlled to maximize the recovery of valuable metals.

*Keywords: Pyrometallurgical processing, recovery, silver, palladium*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 7

November 22

10:50-12:30

# Technical **Oral Session _ Session 7**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 7 (A7)** **10:50 - 12:30, Nov. 22**

**Chair :** Yoon-Uk Heo (Pohang University Of Science And Technology) Halla Hall A, 3F

10:50-11:20 **K-A0817** **[Keynote] The effect of boundaries on the toughness in a high strength low alloy structural steel**
Chengjia Shang (University of Science and Technology Beijing, China)

11:20-11:40 **I-A0787** **[Invited] An original unified approach for the description of phase transformations in steel during cooling**
Olivier Bouaziz (University of Lorraine, France)

11:40-12:00 **I-A0686** **[Invited] Deformation microstructure of pearlitic steel at different conditions**
Rintaro Ueji (National Institute for Materials Science, Japan)

12:00-12:15 **O-A0418** **Comparative study on the role of the grain boundary segregation of phosphorus and sulfur on the hot ductility in low-carbon steel**
Soohyun Kim (Graduated Institute of Ferrous & Materials Technology, POSTECH, Korea)

12:15-12:30 **O-A0030** **Strengthening-Toughening Mechanism of Nitrogen-Containing AISI H13 Steel**
Jie Zhou (Shougang Group, China)

# The effect of boundaries on the toughness in a high strength low alloy structural steel

**Chengjia Shang**[1], Jingxiao Zhao[2]

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## Abstract

High performance low alloy structural steels are widely applied in infrastructure and industries. Increasing the strength of steel is a trend to reduce structural weight, save cost and decrease environmental pressure. However, the increase in strength is always associated with the deterioration in toughness. For the safety of the high-rise buildings, long-span bridges, large container ships and long-distance pipelines, excellent low temperature toughness is required, which is one of the key challenges for the metallurgists. Low carbon bainitic and martensitic phases are dominant microstructure to achieve high strength and high toughness. Prior austenite grain, packet, block and variants constitute the hierarchical microstructure of bainite and martensite. In the present work, crystallographic characteristic of boundaries in low carbon bainitic and martensitic microstructure is investigated to reveal the correlations of chemical composition, prior austenite grain size and cooling rate with the variant selection, boundary density and mechanical properties.

*Keywords: High strength low alloy steel, microstructure characterization, boundaries, martensite/bainite, toughness*

# An original unified approach for the description of phase transformations in steel during cooling

**Olivier Bouaziz** [1,2]

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**Abstract** and

Exploiting Landau's theory of phase transformations, defining an original order parameter using the phenomenological transformation temperatures, it is reported that it is possible to describe in a global approach the conditions for the formation of each phase (ferrite, bainite, martensite) from austenite during cooling in steel. It allowed propose a new rigorous classification of the different thermodynamic conditions controlling each phase transformation. In a second step, the approach predicts naturally the effect of cooling rate on the bainite start temperature.

*Keywords: phase transformation, steel, austenite, ferrite, bainite, martensite, Landau, order parameter.*

# Deformation microstructure of pearlitic steel at different conditions

**Rintaro Ueji**[1], Hidetoshi Somekawa[2], Satoshi Emura[3]

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## Abstract

Pearlite is one of the fundamental microstructures in steel. Thus the change of morphologies and texture in pearlite by deformation should be important for the design of steel microstructure to obtain advanced mechanical properties. This work presented the change in morphology as well as the texture of the pearlitic steels. Spring steel (0.53wt%C-1.48%Si-0.70%Mn-0.76%Cr-Fe) with a pearlitic structure was compressed at various temperatures (room temperature to 600 °C) and various strain rates (0.001 to 1 /sec) to a reduction in height of 30% at maximum. In the specimen compressed at room temperature at 1/sec, X-Ray diffraction measurement of texture clarifies that the deformation texture with a dominant component of <111> in ferrite parallel to the compression axis started evolving at a significantly slight strain of around 10 %, followed by the formation of the firm fiber texture in which <111> parallels preferentially to the compression axis with a maximum intensity of more than ten times random. This significant concentration of orientation brings the plastic anisotropy which was evaluated by the second compression of small specimens which were cut from the first compression with different loading directions having different angles from the first compression axis. In addition to these anisotropies of texture and yield stress, the minor strain rate sensitivity presented by the so-called m-value equal to almost zero brought the kinking lamellar structure because of plastic instability. The compression at hot temperatures revealed that the kinking was suppressed at higher temperatures where the m-value becomes positive adequately.

*Keywords:* steel, pearlite, hot compression, plastic deformation, kinking. texture

# Comparative study on the role of the grain boundary segregation of phosphorus and sulfur on the hot ductility in low-carbon steel

**Soo-Hyun Kim[1],** Sang-Hum Kwon[2], Jae-Sang Lee[3], Yoon-Uk Heo[4*]

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## Abstract

The formation of surface cracks in the slab causes the loss of productivity in the continuous casting process and the cost increase in the final product. There are several origins of surface crack formation in the slab, such as grain boundary (GB) precipitation, ferrite film formation, and impurity segregation. However, which factors govern the crack formation behavior and how the individual factor correlates with each other for crack formation is not clarified. Using the high-temperature tensile test, this study investigates the role of GB segregation of impurities (P, S) to understand the origin of hot-ductility loss in low-carbon steel.

Two equations that explain the GB equilibrium segregation and GB segregation kinetics were used to evaluate impurities' grain boundary segregation behavior. The amount of S segregation was calculated by subtracting the scavenged S contents by MnS formation. Then, the reduced GB decohesion strength by impurity segregation was calculated. The calculated results were compared to the reduction of area (RA) value in the hot tensile test range of 400 to 900°C. The RA curve trend was similar to the reduced grain boundary decohesion strength trend. RA trough was deeper and wider toward high temperature with the S addition. GB segregation of S was quantitatively assessed by EPMA and TEM-EDS. The effect of GB segregation of individual impurities on the hot ductility in low-carbon steel is further discussed.

*Keywords: Hot ductility, Grain boundary segregation, Grain boundary decohesion strength, Intergranular fracture*

# Strengthening-Toughening Mechanism of Nitrogen-Containing AISI H13 STEEL

**Jie Zhou[1],** Yue Ma[1], Qian Tong[1], Naibing Lv[1], Shixin Xu[1]

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**Abstract**

Type or paste your text into this file, and use single-spaced 12-point Times New Roman. Paragraphs are justified (straight-edged) on both left and right. Leave a line gap between paragraphs. The limit for your abstract is 250 words. Do not include tables, formulae, and equations.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: Provide a maximum of 5 keywords which appropriately represent the contents of the presentation.*

# Technical **Oral Session _ Session 7**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 7 (B7)** **10:50 - 11:35, Nov. 22**

**Chair :** Robert Wilson (CSIRO Manufacturing), Hwijun Kim (Korea Institute of Industrial Technology) 301, 3F

10:50-11:20 **K-B0531** **[Keynote] Powders Aren't Powders: Power engineering to wires, composite powders and powder shape control**
Robert Wilson (CSIRO Manufacturing, Australia)

11:20-11:35 **O-B0742** **Effect of cooling rate on the thermoelectric performances of water atomized BiSbTe alloys**
Eun-Ha Go (Kongju National University, Center For Advanced Materials and Parts of Powders CAMP2), Korea)

# Powders Aren't Powders: Power engineering to wires, composite powders and powder shape control

**Robert Wilson[1],** Shiqin Yan[1], Mingshi Song[1], Ling Chen[1], KunYang[1]

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Topic Area: Advanced Processing of Materials Symposium

**Abstract**

The way in which powders and particulates are manufactured, or formed, determines their morphology, particle size distribution (PSD), chemistry and surface condition that in turn dictates their bulk properties such as density, flowability, compactability, etc. The bulk properties of the powders are then critical for allowing them to be further processed into another form such as wire, powder metallurgical or additively manufactured component. These considerations are particularly important when dealing with recycling or repurposing of waste particulates such as machining chips or large gas atomised powders that are not immediately suitable as feeds for component manufacture and are generally bundled and remelted, leading to lost money, time, and energy. CSIRO has developed methods to repurpose both machining chips and large gas atomised particles of grade 23 titanium into feed suitable for wire making via a unique particulate conditioning method and manufacture into wire by a unique wire making methodology. By a similar particulate conditioning method, the chemistry may be additionally tailored to produce composite metal-metal, metal-ceramic particles as well as control the particles' shape to tailor such things as compaction, density, and flow for subsequent processing. This work will detail the repurposing of large gas atomised powders and machining chips as feed to make wires and the wire making process for titanium materials. It will also overview the powder engineering of magnesium for the targeted manufacture of magnesium matrix composites and the shape control of graphite particles for the subsequent targeted fabrication of electrodes in battery systems.

*Keywords: metal powders, powder conditioning, powder metallurgy, additive manufacturing, wire making.*

# Effect of cooling rate on the thermoelectric performances of water atomized BiSbTe alloys

Eun-Ha Go[1], Babu Madavali[1], **Vasudevan Rathinam**[1], Gi-An Song[1], Jin-Kyu Lee[1], Soon-Jik Hong*[1]

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## Abstract

Herein, we report the cooling rate of p-type $Bi_{0.5}Sb_{1.5}Te_3$ (BST) alloys prepared by water atomization and then followed by a spark plasma sintering technique to fabricate the bulk specimen. In particular, the influence of cooling rate on the thermoelectric properties of hot and cold water – BST samples was studied systematically. Initially, water atomized BST powders possess wider particle size distributions with irregular shapes and decreased mean particle size for cold water BST samples. BST alloy exhibits a single phase of R-3m rhombohedral crystal structure and the elementals are distributed homogenously following the stochiometric composition. The fracture surface clearly shows the laminar structure and highly dense microstructure with negligible porosity.

Notably, no observable significant differences in electronic transport properties, besides, a marginal decrement in the lattice thermal conductivity for the cold water- BST. Still, investigations were made to understand the mechanism behind the lowered lattice thermal conductivity for cold water-BST?. The thermal conductivity of BST follows the Umklapp scattering phenomena in the low-temperature region and then experiences bipolar conduction at higher temperatures due to its narrow energy band gap ($E_g$). With the contribution of lower thermal conductivity (~0.9 W. $m^{-1}K^{-1}$), the cold water - BST shows substantially higher $ZT_{max.}$ of 1.3 at 400 °C. Hence, this study reveals that the water-atomization would be cost-effective to prepare a bulk BST without using expensive inert gases and also, scalable to mass production for industrial purposes in the future.

*Keywords*: BiSbTe alloy, water atomization, cooling rate, spark plasma sintering, thermal conductivity

# Technical **Oral Session _ Session 7**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 7 (C7)** **10:50 - 12:10, Nov. 22**

Chair : Masatoshi Mitsuhara (Kyushu University), Longfei LI (University of Science and Technology Beijing) 201A, 2F

10:50-11:20 **K-C0883** **[Keynote] Recrystalization and phase transformations in metastable beta titanium alloys**
Elena Pereloma (University of Wollongong, Australia)

11:20-11:40 **I-C0271** **[Invited] Microstructure and mechanical properties of TiAl alloys fabricated by electron beam powder bed fusion**
Hiroyuki Yasuda (Osaka University, Japan)

11:40-11:55 **O-C0142** **Thermal deformation mechanism and low-temperature superplasticity of β-stabilized Ti-43Al-9V-Y alloy sheet with bimodal γ -grain-size distribution**
Yu Zhang (Harbin Institute Of Technology, China)

11:55-12:10 **O-C0844** **Fracture Toughness of γ-TiAl from First-Principles Calculations**
Mahfooz Alam (Indian Institute of Technology Jodhpur, India)

# Recrystalization and phase transformations in metastable beta titanium alloys

**Elena Pereloma**[1]

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## Abstract

Metastable beta Ti alloys are important structural materials. During their production and in-service they are subjected to high temperatures and deformation. Thus, understanding of the evolution of microstructure under these external conditions is important for fine-tuning their properties for various applications.

In this presentation, some aspects of the beta phase recrystallization and decomposition with formation of alpha phase will be discussed. In addition, a complex deformation behaviour at elevated and ambient temperatures will be addressed. Advanced experimental techniques, such as electron back-scattering diffraction, scanning transmission electron microscopy and atom probe tomography were utilized to gain insight in the phenomena.

*Keywords: metastable β Titanium alloys, recrystallization, aging, electron microscopy, atom probe tomography.*

# Microstructure and mechanical properties of TiAl alloys fabricated by electron beam powder bed fusion

**Hiroyuki Y. Yasuda**[1], Ken Cho[2], Mitsuharu Todai[3], Masao Takeyama[4], Takayoshi Nakano[5]

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## Abstract

TiAl alloys have been used for low pressure turbine blades of aircraft jet engine due to lightweight, high temperature strength and good oxidation resistance. Recently, additive manufacturing of TiAl alloys has attracted much attention since the process is near-net shape, mold-free and done in vacuum, which is suitable for the fabrication of TiAl alloys. In the present study, Ti-48Al-2Cr-2Nb and Ti-44Al-4Cr (at.%) alloys were fabricated by an electron beam powder bed fusion (EB-PBF) which is one of typical additive manufacturing processes. Microstructure of TiAl alloys is found to be very sensitive to an energy density calculated from beam current, scanning speed and scanning pitch. For instance, in Ti-48Al-2Cr-2Nb alloys, unique banded structure composed of the duplex structure and a chain of γ grains (γ band), which is closely related to the temperature distribution near the melt pool created by an electron beam. If the angle between the tensile axis and γ bands is 45°, large elongation above 2.5% can be obtained even at room temperature. In contrast to Ti-28Al-2Cr-2Nb alloys, Ti-44Al-4Cr alloys contain the β phase, together with the $\alpha_2$ and γ phases. In Ti-44Al-4Cr alloys, massive transformation from the β to α phase takes place at low energy densities, followed by the formation on ultra-fine lamellar structure consisting of the $\alpha_2$ and γ phases. Ultra-fine lamellar grains contribute to high temperature strength through the Hall-Petch law. Thus, the microstructure and mechanical properties of TiAl alloys can be controlled by additive manufacturing.

*Keywords: Additive manufacturing, Titanium aluminides, Intermetallics, High temperature structural materials*

# Thermal deformation mechanism and low-temperature superplasticity of β-stabilized Ti-43Al-9V-Y alloy sheet with bimodal γ -grain-size distribution

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## Abstract

The deformation mechanism and superplasticity of Ti-43Al-9V-0.2Y alloy sheet hot-rolled at 1100 °C was systematically investigated. Due to its special c/a axial ratio, polyphase characteristics and complexity of the phase diagram of TiAl alloys, various transformation modes and interfaces appear during hot-rolling, such as γ/$\alpha_2$ lamellar, f.c.c → $L1_0$ ordering process, α → γ massive-type transformation, etc. A bimodal γ grain distribution microstructure of this TiAl alloy sheet, with abundant nano-scale or sub-micron γ laths embedded inside β matrix, exhibits an impressive superplastic behaviour. This inhomogeneous microstructure shows low-temperature superplasticity with a strain-rate sensitivity exponent of m = 0.27 at 800 °C, which is the lowest temperature of superplastic deformation for TiAl alloys attained so far. The maximum elongation reaches ~360% at 900 °C with an initial strain rate of $2.0 \times 10^{-4}$ $s^{-1}$. The results of in situ high-temperature X-ray diffraction (XRD) indicate that β phase does not undergo the transformation from an ordered $L2_0$ structure to a disordered *A2* structure and cannot coordinate superplastic deformation as a lubricant. This superplastic deformation mechanism can be explained by the combination of DR and grain boundary slipping (GBS). In the early stage of superplastic deformation, DR is an important coordination mechanism as associated with the reduced cavitation and dislocation density with increasing tensile temperature. At the late stage of superplastic deformation, these equiaxed grains make GBS prevalent, which can effectively avoid intergranular cracking and is conducive to the further improvement in elongation.

*Keywords: Titanium aluminides, Hot-rolled alloy sheet, deformation mechanism, superplasticity,*

# Fracture Toughness of γ-TiAl from First-Principles Calculations

**Mahfooz Alam**[1], Appala Naidu Gandi[1]

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**Abstract**

γ-TiAl is considered for aerospace applications due to its low density, high melting temperature, high strength, and modulus retention at elevated temperatures. But the main drawback of this material is the low fracture toughness, limiting its applications. Accurate models that can predict fracture toughness aid in better materials design. A recently proposed model expresses the fracture toughness $K_{IC}$ as an empirical relation of bulk modulus, shear modulus, atomic volume, the density of states, and electronegativity. This model predicts the room temperature $K_{IC}$ values for covalent crystals, ionic crystals, metals, and alloys. $K_{IC}$ variation with temperature in γ-TiAl has been studied using the first-principles calculations and quasi-harmonic approximation to investigate the accuracy of the model for determining the high-temperature fracture toughness. The predicted $K_{IC}$ value of 8.34 MPa√m at 300 K agrees well with the experimental value of 8.6 MPa√m. Estimated $K_{IC}$ values decrease with the increase in the temperature, whereas the experimental $K_{IC}$ values increase slightly with the increase in the temperature. Estimated bulk modulus and shear modulus values are decreasing with the increase in temperature, as expected experimentally. The atomic volume and density of states are not changing much with the temperature within the quasi-harmonic approximation. The electronegativity values are fixed for a given element. Therefore, the existing model inherently predicts a decrease in fracture toughness with an increase in temperature. However, experimentally the fracture toughness increases with the temperature in TiAl samples. Therefore, additional model parameters should be included to incorporate the temperature effect.

*Keywords: Fracture toughness, stiffness tensor, quasi-harmonic approximation, first-principles calculations.*

# Technical **Oral Session _ Session 7**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 7 (D7)** **10:50 - 12:10, Nov. 22**

**Chair :** Mingzhe Bian (AIST), Jun Ho Bae (Korea Institute of Materials Science) Samda Hall A, 3F

10:50-11:10 **I-D0561** **[Invited] Additive Manufacturing of Mg alloy WE43 by Directed Energy Deposition**
Cherry Chen (CSIRO Manufacturing, Australia)

11:10-11:25 **O-D0189** **Effects of different wrought processes on microstructure evolution and mechanical properties of AZ31 magnesium alloy**
Hiromasa Yoshizumi (Doshisha University, Japan)

11:25-11:40 **O-D0656** **Micro backward extrusion of Light weight Magnesium alloys**
VENKATESH BEHERA (Indian Institute Of Technology Madras,India)

11:40-11:55 **O-D0921** **Simultaneous improvement in strength and ductility of extruded AZ91 alloy by utilizing ultrasonic nano-crystalline surface modification (UNSM) treatment**
Hyun Ji Kim (Kyungpook National University, Korea)

11:55-12:10 **O-D0071** **Effect of extrusion temperature on the microstructure, mechanical properties, and cavitation behavior of Mg-0.8Mn (wt%) alloy**
ChongChao Li (Pohang University of Science and Technology, Korea)

# Additive Manufacturing of Mg alloy WE43 by Directed Energy Deposition

Mingshi Song[1], **Ling Chen[1]**, Robert Wilson[1], Kun Yang[1], Timothy Hughes[1], Helmut Thissen[1], Xiaobo Chen[2]

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## Abstract

Magnesium (Mg)/Mg alloys, with their degradable nature and comparable mechanical properties to those of human bone, show their potential as temporary bone substitutes which will degrade with the restoration of the bone defect, without the need for a secondary surgery to remove them. Three-dimensional (3D) printing has become one of the most revolutionary and powerful manufacturing tools, allowing the fabrication of patient specific complex porous structures, which is favourable for nutrient transfer and metabolites exchange and will be highly demanded in the future. There is a growing interest from both academia and industry in the 3D printing of Mg and its alloys. Many additive manufacturing (AM) technologies, such as powder bed fusion, wire arc AM, pate extrusion deposition, friction stir AM and binder jet have been used to demonstrate the feasibility of Mg 3D printing. However, it remains a challenge to 3D print Mg alloy parts/components in high quality because of the low printability of Mg, which is due to its inherent flammability, high chemical reactivity, and small difference between its melting and vaporisation temperatures.

This work for the first time, employs a different AM technology, a directed energy deposition (DED) process to build porous Mg alloy WE43 structures. A few porous Mg alloy structures with different umbers of pores and pore sizes were fabricated. Printability, geometry accuracy, build defects and microstructures were analysed. How the printing parameters affect those properties were explored. This work is expected to inspire future research on 3D printing of Mg based materials.

*Keywords: Light Metals, Magnesium Alloys, Additive Manufacturing, Directed Energy Deposition, Microstructure.*

# Effects of different wrought processes on microstructure evolution and mechanical properties of AZ31 magnesium alloy

**Hiromasa Yoshizumi[1,4],** Motohiro Yuasa[2,4], Hiroyuki Miyamoto[3], Hidetoshi Somekawa[4]

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## Abstract

AZ31 magnesium alloy was processed by five wrought processes (forging, rolling, extrusion, equal-channel-angular-extrusion (ECAE), and, caliber rolling) at 573 K. The applied strain in these processes was unified to approximately 1.5. The introduced strain was computed with the finite element method (FEM). Although the same equivalent plastic strain was induced, various microstructures and textures were observed by electron back-scattering diffraction (EBSD). A combination of calculation and observation shows that the basal texture aligns perpendicular to the compressive strain and the intensity of this texture develops with the increase of compressive strain. The forging and rolling, which introduce compressive strain in one direction, form stronger basal texture than the other processes such as caliber rolling, which induce compression in multi-direction. The strain state also influences the microstructure. During the multi-directional compression, the more refined and homogeneous microstructure evolved than the uniaxial compression.

The mechanical property was investigated by a tensile test at room temperature. 0.2 % proof stress was increased with grain refinement, according to the Hall-Petch relationship. The rolled alloy and extruded had similar grain sizes, but the proof stress of the former was higher by approximately 50 MPa than the latter. This is attributed to the strengthening by the intensive basal texture. The forged alloy, whose average grain size was twice as large as that of rolled, also had intensive texture, yet the strengthening by texture was not significantly shown. This suggests that the degree of strengthening by the texture depends on the grain size.

*Keywords: Magnesium alloy, Dynamic recrystallization, Texture, Finite element method, Mechanical property.*

# Micro backward extrusion of Light weight Magnesium alloys.

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Product miniaturization is the current need of various industrial sectors and hence micro component manufacturing is the recent need in several applications including bio-medical, aerospace, micro-electromechanical systems (MEMS) etc. Being the lightest weight structural material, Mg alloys find their suitability in micro component application domain. Among several micro manufacturing processes, micro extrusion process is a promising method to develop micro components. However, micro extrusion is a plastic deformation process and Mg alloys cannot be extruded at room temperature due to their inherent HCP crystal structure. Therefore, it is essential to develop a high temperature equipped micro-extrusion technology to extrude materials which are difficult to deform at room temperature. The complex tool design of a micro-extrusion tool cannot be accomplished by just scaling down the existing macro scale extrusion technology to micro scale domain. Also, the tool design has a crucial role deciding the dimensional accuracy, surface finish, repeatability, defects etc., of the manufactured micro-component.

The present study is focussed on establishing the backward micro extrusion behaviour of a rare earth contained Mg alloy at varying temperature domain. This study includes micro extrusion tool development, detailed experimentation and structure-micro extrusion correlation. The scientific knowhow of microscale deformation behaviour and micro mechanics during micro extrusion process at varying temperature and process parameters are established in this work via detailed microstructural characterization including FESEM, EBSD, TEM tools etc.

*Keywords: Magnesium alloys, Light weight, Micro-extrusion.*

# Simultaneous improvement in strength and ductility of extruded AZ91 alloy by utilizing ultrasonic nano-crystalline surface modification (UNSM) treatment

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Mg alloys have great potential as lightweight structural materials due to their low density, but their application is limited because of the lower mechanical properties comparing to the other lightweight alloys. In order to increase a competitiveness as structural metal material, studies to develop Mg alloys with improved strength and ductility at the same time has been actively investigated. Recently, there has been a few research which is undergoing to improve the mechanical properties by introducing a gradient structure to obtain a good balance of mechanical properties such as strength and ductility. Ultrasonic nano-crystalline surface modification (UNSM) technique, which induces severe plastic deformation on the material surface using ultrasonic impact, can result in the gradient microstructure with refined surface consisted of nano-sized grains and intermediate microstructure with residual strain. While the nanocrystalline surface contribute to improve strength and ductility, the residual strain in the intermediate microstructure bring out a significant reduction in ductility. However, the residual strain can be beneficial for both strength and ductility through recovery, recrystallization or strain-induced precipitation according to an appropriate annealing treatment. In this study, we applied the UNSM treatment and subsequent annealing at 200 °C to a homogenized AZ91 alloy extrudate to improve strength and ductility at the same time by generating the gradient microstructure. Microstructural and mechanical properties were analysed by using an electron backscatter diffraction (EBSD), scanning electron microscopy (SEM), Vickers hardness tester, and tensile testing machine.

*Keywords: AZ91 alloy; UNSM(Ultrasonic Nano-Crystalline Surface Modification); Gradient microstructure; Annealing treatment; Mechanical properties.*

# Effect of extrusion temperature on the microstructure, mechanical properties, and cavitation behavior of Mg-0.8Mn (wt%) alloy

**ChongChao Li** [1], XiaoGuang Qiao [2], MingYi Zheng [3, **], Hyoung Seop Kim [4, *]

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## Abstract

The microstructure, superior ductility, and evolution of cavities at room temperature in as-extruded Mg-0.8Mn (M08, wt%) alloy with different extrusion temperatures were investigated. The M08 alloy extruded at 150 ℃ exhibits a bimodal structure and extruded at 210 °C exhibits fully dynamic recrystallized (DRXed) grains. At the same time, the grains grow as the extrusion temperature increases. The grain boundary segregation will decrease and more precipitates are created with the high extrusion temperature. The ductility of the fine-grained M08 sample is 74% at a strain rate $1.0\text{x}10^{-3}$ $s^{-1}$. The high strain rate sensitivity exponent ($m$-value, 0.16) implies grain boundary sliding plays an important contribution to plastic deformation in fine-grained M08 alloy. Conversely, the M08 alloy extruded at 300 °C with a low $m$-value (0.009) exhibits a poor ductility of 16%. The cavities are mainly initiated at the (trigonal-) grain boundaries, and the mechanism of cavities growth in the as-extruded M08 alloy is controlled by plasticity. The growth parameter ($\eta$-value) in the M08 alloy extruded at 300 ℃ is 3.1, which is slightly higher than that in the fine-grained M08 alloy with $\eta = 2.5$.

***Keywords:*** Mg-0.8Mn alloy; Extrusion; Superior ductility; Grain boundary segregation; Cavitation behavior

# Technical **Oral Session _ Session 7**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 7 (E7)** **10:50 - 12:30, Nov. 22**

**Chair :** Daisuke EGUSA (The University of Tokyo) Halla Hall B, 3F

10:50-11:20 **K-E0426** **[Keynote] Materials Integration for Additive Manufacturing**
Makoto WATANABE (National Institute for Materials Science, Japan)

11:20-11:40 **I-E0458** **[Invited] Research progress of graded alloy fabricated by additive manufacturing**
Zhang Baicheng (University of Science and Technology Beijing, China)

11:40-12:00 **I-E1136** **[Invited] Research progress of graded alloy fabricated by additive manufacturing**
Mahyar Khorasani (Royal Melbourne Institute of Technology, Australia)

12:00-12:15 **O-E0395** **ADefect evaluation during metal additive manufacturing by AE method and machine learning**
Gaku Ito (The University of Tokyo, Japan)

12:15-12:30 **O-E0929** **Experimental investigation of DLP 3D-printed Ti-6Al-4V**
Chang Woo Gal (Korea Institute of Materials Science, Korea)

# Materials Integration for Additive Manufacturing

**Makoto Watanabe**[1]

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**Abstract**

Additive manufacturing is a process that directly builds three-dimensional structures by layering materials according to computer-aided design. It enables the production of components with complex shapes that are difficult to produce using conventional technologies, as well as reducing the number of parts by manufacturing them as a single component. It is expected to be used increasingly in the aerospace and energy industries, where high quality products are required in small quantities. When applying this process to the production of high-performance heat resistant alloy components, it is important to control the occurrence of defects during the process and to optimize the microstructure and mechanical properties. Therefore, the selection or development of materials suitable for the additive manufacturing process and the optimization of process conditions are key. Since the development of new materials has traditionally required long-term research, there are great expectations for shortening the development time through the use of computation. In our research, we call the predictive technology combining various simulations and data science "materials integration", and we have developed various simulation techniques and data science for the laser powder bed fusion process, designed new heat-resistant alloys by applying these techniques, and developed monitoring techniques to validate these predictions. This talk will provide a comprehensive overview of these achievements.

*Keywords: Additive Manufacturing, Laser Powder Bed Fusion, Multi-physics Simulation, Process Monitoring, Alloy Design.*

# Research progress of graded alloy fabricated by additive manufacturing

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**Abstract**

Continuous graded alloy fabrication by LPBF (Laser Powder Bed Fusion) is a new technique in additive manufacturing that allow to create alloys with varying compositions and properties in a single part. Recent studies have shown promising results in creating continuous graded alloys with improved mechanical, thermal, and corrosion resistance properties, which can be applied in various industries such as aerospace, biomedical, and automotive. Speaker will give a comprehensive introduction of the controlling the composition gradient, modifying the laser scan strategy, microstructure and mechanical properties evolution.

*Keywords: laser powder bed fusion; high throughput; graded alloy.*

# High Fidelity Simulation of Meltpool Phenomena in Laser-Based Powder Bed Fusion of Inconel 718

**Mahyar Khorasani [1,2]**, Martin Leary[1], Stuart Bateman[1],
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**Abstract**

In this investigation, the effective and driving factors on meltpool of Laser-Based Powder Bed Fusion (LB-PBF) such as optical penetration depth, angle of incidence, the ratio of laser power to scan speed, surface properties, and plasma formation are discussed. The contribution of this work is characterising the fundamental governing factors on meltpool depth and developing an analytical model based on process parameters and powder properties. The proposed model helps to accurately predict the meltpool depth which is important and has to be sufficient to effectively fuse the powder to the build plate or the previously solidified layers ensuring proper bonding quality. The model is useful to estimate the meltpool depth for various manufacturing conditions. A proposed methodology is based on the high-fidelity simulation of a set of process parameters to obtain the variation of meltpool depth and temperature, followed by validation with reference to experimental test data. Numerical simulation of the LB-PBF process was implemented using the computational fluid dynamic (CFD) tool "Flow-3D Version 12" to obtain the meltpool features. The simulation data was then developed into a predictive analytical model for meltpool depth and temperature based on the thermophysical powder properties and associated parameters. Results showed that the developed analytical model has a high accuracy to predict the meltpool depth. The model is useful to rapidly estimate the optimal process window before setting up the manufacturing tasks and can therefore save on lead-time and cost. The discussions identified how the effective physical factors govern the induced heat versus meltpool depth which can affect the bonding and the quality of the components.

*Keywords: Additive Manufacturing, Laser-Based Powder Bed Fusion, Meltpool Depth, High Fidelity Simulation, Computational Fluid Dynamics.*

# Defect evaluation during metal additive manufacturing by AE method and machine learning

**Gaku Ito[1],** Kaita Ito[2], Masahiro Kusano[3], Takayuki Shiraiwa[1], Makoto Watanabe[3], Manabu Enoki[1]

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**Abstract**

Laser Powder Bed Fusion (LPBF) is an additive manufacturing process that uses a laser as a heat source and is being researched and developed as a new manufacturing process for high-strength, difficult-to-process materials. The acoustic emission (AE) method detects elastic waves emitted when a material is broken or deformed It detects the time, location, and magnitude of the events in real time. In our previous study, by comparing the X-ray CT image of a molding object with the measured AE waveform, it was found that there is a correspondence between defects generated during the process and AE events.

In this study, we aimed to identify the types of defects during LPBF processing using the AE method by measuring the AE signals generated by single-layer fabrication and performing machine learning. Ni-based superalloy Inconel738LC was used as the material. Molding was performed under different conditions of generated defects by changing molding parameters such as laser output and scanning interval, and AE signals generated during molding were measured and analyzed. In order to use the measured AE signals as input data for a convolutional neural network (CNN), the AE signals was transformed into a time-frequency spectrum by a short-time Fourier transform (STFT). As a result, we were able to classify each molding condition with an accuracy of 95% or more. In addition, it was found that learning was performed with attention paid to the high-frequency band in response to the occurrence of cracks, especially under high laser output conditions.

*Keywords: laser powder bed fusion, additive manufacturing, acoustic emission, machine learning, convolutional neural network*

# Experimental investigation of DLP 3D-printed Ti-6Al-4V

**Chang Woo Gal[1],** Yeong-Jin Choi[1], Honghyun Park[1], Aram Sung[1], Hui-suk Yun[1,2]

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## Abstract

Digital light processing (DLP) technology has emerged as an attractive additive manufacturing method because of its numerous advantages in terms of shape complexity, low surface roughness, realization of fine details, and so on. However, applying DLP to metallic materials presents challenges when it comes achieving sufficient curing ability of metal slurry and maintaining slurry stability during printing. In this study, we investigated DLP printing with Ti-6Al-4V to overcome these challenges and realize metal printing. First, we sought to enhance the curing ability by classifying the raw powders. Then, we designed a resin system for the metal slurry to minimize metal powder sedimentation, analyzing the rheological and sedimentation behavior. The designed resin system showed acceptable printing viscosity and printability. The DLP 3D-printed Ti-6Al-4V structures demonstrated good interlayer bonding without any defects. Subsequently, the thermal debinding behaviour of Ti-6Al-4V under temperature and debinding atmosphere conditions and sintering of Ti-6Al-4V in a vacuum furnace were analysed, supported by carbon- and oxygen-level examinations.

*Keywords: Ti-6Al-4V, Digital light processing, UV-curable suspension, Debinding, Sintering*

# Technical **Oral Session _ Session 7**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 7 (F7)** **10:50 - 12:30, Nov. 22**

**Chair :** Tingting Song (RMIT University), Qiyang Tan (Architecture and Information Technology) 202A, 2F

10:50-11:20 **K-F0269** **[Keynote] 3D microstructural analysis of electroless Ni-P-plated Al-Zn-Mg alloys**
Keitaro HORIKAWA (Osaka University, Japan)

11:20-11:40 **I-F0871** **[Invited] Nano-pyramid metallic coating for ultraselective and ultrapermeable separation membranes for oil/water emulsions**
Jinn P. Chu (National Taiwan University of Science and Technology, Taiwan)

11:40-12:00 **I-F1028** **[Invited] Novel thermal environmental barrier coatings used at ultra-high temperatures**
Jian He (Beihang University, China)

12:00-12:15 **O-F0010** **Study on the cause and mechanism of the stripe color difference defects of cold-rolled duplex steel galvanized strip**
Wang Chang (Shougang Research Institute of Technology, China)

12:15-12:30 **O-F1129** **Surface Engineering of Metal Nanocrystal Thin Films for flexible and high-performance electromagnetic interference shielding materials**
Seoyeon Park (Korea University, Korea)

# 3D microstructural analysis of electroless Ni-P-plated Al-Zn-Mg alloys by means of synchrotron X-ray CT and dynamic hydrogen detection

**Keitaro Horikawa**[1], Makoto Hino[2], Kazuyuki Shimizu[3], Hiroyuki Toda[4], Masato Hoshino[5] and Kentaro Uesugi[6]

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## Abstract

The internal microstructure of Ni-P-plated Al-Zn-Mg base alloys near the surface region was studied through synchrotron X-ray computed tomography (CT). The X-ray energy of 40 keV was used and the voxel size was 0.78 μm. The CT imaging was performed by rotating the specimen 180 degrees on the stage during the test (exposure time of 60 msec/frame, 3600 images/180 degrees). 3D reconstruction of the 2D tomographic images was carried out using the rendering software Amira3D. After the observation, slow strain rate tensile testing was performed at a crosshead speed of 0.005 mm/min, together with dynamic hydrogen detection using gas chromatography in the closed chamber under an ambient air atmosphere.
It was shown that hydrogen micropores were generated and segregated near the surface region in the commercial purity graded 7075-T6 aluminum alloys with Ni-P plating. In contrast, such segregation of hydrogen micropores was not observed in the 7075-T6 alloys without Ni-P plating or in high-purity-based alloys. This suggests that hydrogen entered the Ni-P plating layer during the plating operation generating micropores at the surface region depending on the purity of test alloys.

*Keywords: Aluminum Alloy, Ni-P Plating, Synchrotron X-ray CT, Hydrogen Micro-pore, Dynamic Hydrogen Detection*

# Nano-pyramid metallic coating for ultraselective and ultrapermeable separation membranes for oil/water emulsions

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## Abstract

In this presentation, the stainless-steel (SS) nano-pyramid structure with many unique properties is first presented. This SS coating is sputter-deposited on various substrates. Particularly, we applied for the first time this SS nano-pyramid structure on mixed cellulose ester (MCE) membrane for the use in separation of oil/water emulsions. SS-coated MCE membrane presented a superhydrophilic, antifouling surface and underwater superoleophobicity. The coated membrane showed excellent separation efficiency of >99% when applied to light oil-water emulsions with a range of viscosities and densities. The highest permeation flux measured was 1,555 litre/$m^2$/hr when applied to toluene-in-water emulsions, outperforming by 2-fold all other membranes. The coated membrane was shown to work well under harsh conditions including salty water, extreme pH values (1 to 14) and high temperatures (60 °C). The membrane also presented outstanding recyclability, as evidenced by oil rejection rate retaining at >99% through four separation cycles. In addition, our fabrication route of SS-coated MCE employs low-process temperature while being highly scalable, which is favorable for industrial scale applications.

The author acknowledges many co-workers for their contributions: Mr. Yi-Jui Yeh, Mr. Jhen-De You, Mr. Jr Rong Liou, and Professor Kuo-Lun Tung of NTU, Mr. Ting-Hao Chang and Professor Wei-Hung Chiang of NTUST, Professor Pakman Yiu of MUT, and Professor Yu-Lin Shen of UNM.

*Keywords: oil-in-water emulsion separation, nano-pyramidal structure, stainless steel coating, sputter deposition, superhydrophilicity, underwater superoleophobicity*

# Novel thermal environmental barrier coatings used at ultra-high temperatures

**Jian He[1,3],** Wenting He[2,3], Liangliang Wei[1,3], Hui Peng[1,3], Hongbo Guo[2,3]

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## Abstract

SiC-based ceramic matrix composites (CMCs) have emerged as one of the most promising alternatives for superalloys applied in next-generation gas turbines. But CMCs cannot be used alone in steam environments generated by fuel combustion. Therefore, environmental barrier coatings (EBCs) become indispensable for the application of CMCs which can protect CMCs from the steam corrosion. However, as the thrust-to-weight ratio of the aero-engine continues to improve, the turbine inlet temperature is getting much higher. The traditional EBCs composed of Si bond coat and rare earth (RE) silicates top coat cannot meet the application requirements at ultra-high temperatures. Adding a thermal barrier layer on EBCs to form thermal environmental barrier coatings (TEBCs) is an effective solution. Accordingly in our recent work, RE zirconates, RE phosphates and yttria stabilized hafnia were designed as thermal barrier materials and added onto EBCs respectively. The preparation of the composite coatings by plasma spray-physical vapor deposition (PS-PVD) combined with air plasma spraying (APS) was investigated. The high-temperature oxidation and steam corrosion behaviour were evaluated and the failure mechanisms were clarified. In summary, the three types of TEBCs showed good oxidation and steam corrosion resistance and PS-PVD contributed to the high crystallinity and high density of EBCs.

*Keywords: Thermal environmental barrier coatings, Preparation, High-temperature oxidation, Steam corrosion, Failure mechanism.*

# Study on the cause and mechanism of the stripe color difference defects of cold-rolled duplex steel galvanized strip

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## Abstract

The causes and mechanism of the strip color difference defects of cold rolled DP590 after galvanized were studied.SEM and EPMA were used to study the morphological characteristics of color difference defects, and the spacing characteristics of banded color difference defects were analyzed through production line tracking. The oxidation characteristics of DP590 steel was analyzed by differential thermal analyzer. It was found that the change of oxidation weight gain rate was related to the interfacial enrichment of Al element and the melting of FeO-$SiO_2$-$Al_2O_3$. The results show that the formation mechanism of strip color difference defects on DP590 galvanized strip surface is as follows: the overlapped area of high-pressure water on strip surface is local supercooling in the process of finishing rolling descaling, and the temperature difference between color difference areas and other areas may reach 100 ℃ due to the effect of other cooling systems (frame cooling water, dust suppression water, roll gap cooling water, etc.) in the hot rolling process. In addition, due to the addition of Si、Al element in the steel, the composite olivine phase of Si、Al element forming at the interface will reduce the heat conduction. The influence of Si、Al composite olivine phase cannot be completely recovered in the supercooling zone, and the deformation ability of the scale is lower in the hot rolling process. With the rolling progress, the cracking risk of the scale in the supercooling zone is increased. In the process of finishing rolling, the strip scales are pressed into steel plate surface and form color difference defects.

*Keywords: Duplex steel; Oxidation characteristics; Al element enrichment; Descaling water overlapping area; Scale pressing defects*

# Surface Engineering of Metal Nanocrystal Thin Films for flexible and high-performance electromagnetic interference shielding materials

**Seoyeon Park[1],** Soongju Oh[2], Jihyuk Choi[3]

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## Abstract

The extensive use of electrical equipment in wearable smart electronics has raised significant concerns regarding electromagnetic interference (EMI). Thus, there is a growing demand for flexible electrodes with versatile EMI shielding capabilities. Among the many candidates for EMI shielding, inorganic colloidal nanocrystals (NCs) have recently emerged as promising candidates for solution-processable materials due to their advantageous physical and chemical properties. In addition, the optical and electronic properties of NC films can be easily engineered by modifying the surface chemistry of NCs through post-synthesis chemical treatment. Here, the highly conductive and flexible thin films exhibiting exceptional EMI shielding properties were successfully studied. These films can be fabricated at room-temperature using colloidal Ag NCs. The preparation of Ag NC films involves a straightforward Layer-by-Layer method that includes ligand exchange and reduction steps. The ligand-exchange process promotes intensive metallic-fusion of Ag NCs to form large-scale and extensive conduction pathways, and the subsequent reduction process further enhances charge transfer within the films by removing non-metallic compounds. Benefiting from their ease of processing, the resulting Ag NC thin films demonstrated a maximum EMI shielding effectiveness (SE) of approximately 60 dB, with a thickness of around 1.3 μm, while maintaining excellent mechanical stability under various deformation conditions.

*Keywords: Nanocrystal, Ligand exchange, Flexible device, Electromagnetic inference shielding*

# Technical **Oral Session _ Session 7**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 7 (G7)** **10:50 - 12:30, Nov. 22**

**Chair :** Dong-Hwa Seo (Korea Advanced Institute of Science and Technology) 303A, 3F

10:50-11:20 **K-G0245** **[Keynote] Enabling scalable high-areal-capacity Li battery cathodes by coupled ion/electron transport**
Sang-Young Lee (Yonsei University, Korea)

11:20-11:40 **I-G1065** **[Invited] How interfaces control lithium (de)insertion pathway**
Jongwoo Lim (Seoul National University, Korea)

11:40-12:00 **I-G0784** **[Invited] Advanced Metal-Based Anode Materials for Li Storage**
Renzong Hu (South China University of Technology, China)

12:00-12:15 **O-G0990** **The synergy between cation and ligand tailors in layered cathodes for highly reversible Li intercalation**
Jiliang Zhang (Dalian Jiaotong University, China)

12:15-12:30 **O-G0962** **Nanoporous Li4Ti5O12 as anode material of Li-ion batteries for excellent high-rate performance**
Zhangjie Xu (Dalian Jiaotong University, China)

# Enabling scalable high-areal-capacity Li battery cathodes by coupled ion/electron transport

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## Abstract

Achieving high-energy-density Li batteries is of primary importance in facilitating the advent of smart energy era. Major research approaches implemented to achieve this goal have focused on the synthesis and modification of electrode active materials and electrolytes. Along with these materials-based works, much attention should be devoted to designing high-areal-capacity electrodes as a facile and scalable architectural strategy. A formidable challenge facing the high-areal-capacity electrodes is the inhomogeneous redox reaction in their through-thickness direction, which stems from poorly-developed ion/electron conduction pathways.

To address this issue, herein, we design a class of practical cathode sheets with focus on coupled ion/electron transport phenomena, which include the heteronanomat-structured cathodes comprising the carbon nanotubes and polymeric nanofibers, ion/electron conduction network-embedded quasi-solid-state electrodes, amphiphilic bottlebrush polymeric binders, and electrostatic polymeric binders. This new cathode architecture strategy presented herein opens a new route toward scalable high-areal-capacity cathodes with redox homogeneity in the through-thickness direction, which lie far beyond those achievable with previously reported conventional cathode sheets based on slurry casting methods.

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*Keywords: Li batteries, Electrodes, High-areal-capacity, Ion/electron transport, Binders*

| I-G1065 |

## How interfaces control lithium (de)insertion pathway

In the realm of lithium-ion batteries, the process of lithium (de)insertion follows a two-fold pathway, encompassing (1) charge transfer occurring at the electrolyte-electrode interface and (2) solid-state lithium diffusion within electrode. Historically, these two transport mechanisms have been regarded as distinct and investigated separately due to their sequential occurrence during battery cycling. However, our recent research demonstrates that the kinetics of charge transfer can excert control over the spatial distribution of lithium on the surface, consequently influencing the entire lithium (de)insertion pathway. In addition, the chemical composition of electrolyte can further modulate the surface charge transfer kinetics, consequently leading to significant alterartion in spatiodynamics of lithium (de)insertion.

# Advanced Metal-Based Anode Materials for Li Storage

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## Abstract

The energy density of LIBs is mainly determined by the voltage difference (V) between the cathode and anode, and in particular, the specific capacity of the electrode materials in suitable potential window. Thus, intense efforts have been devoted to developing high-voltage cathode materials and exploring new high-capacity metal-based (Sn-, Si-, Sb-) anode materials to replace the commercial graphite anode that has a low theoretical specific capacity of 372 mAh $g^{-1}$. In particular, the moderated lithiation potential of metal-based anodes could prevent the Li deposition and dendrite growth and thus could be benefit to fast-charging LIB at subzero-temperatures.

In this presentation, we will discuss the lithation-delithiation behaviours of Sn, InSb, $SnO_2$ and $SiO_x$ at both room- and subzero-temperatures. It was revealed that the reaction mechanism, Li-ion diffusion kinetics, and polycrystalline sphalerite structure of the InSb anode materials remain unchanged during the charging and discharging process at both room and sub-zero temperatures. And subzero temperature can promote stable lithium storage in $SnO_2$, while the LiF-modified $SnO_2$ anodes matched with suitable electrolytes can qualify the LIBs for a safe and long-life at wide temperature (-50~60°C), which is helpful to further promote these batteries for low-temperature applications.

In addition, we will also discuss the strategies to improve the reversibility of conversion reactions and initial Coulombic efficiencies of $SnO_2$ and $SiO_x$-based anodes, and the efforts on reducing voltage hysteresis of metal oxide anodes to achieve high energy efficiency for Li-ion batteries, with the assistance of plasma milling.

*Keywords: Li-ion batteries, Tin-based anodes, Conversion reactions, Voltage hysteresis, Low-temperature*

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# The synergy between cation and ligand tailors in layered cathodes for highly reversible Li intercalation

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## Abstract

Doping could effectively tune the electrochemical performance of layered oxide cathodes in Li-ion batteries, whereas the working mechanism is usually oversimplified (*i.e.,* a 'pillar' effect). Although the Jahn-Teller effect is generally regarded as the fundamental origin of structural instability in some oxides, the pseudo-JTE (PJTE) is actually more common since it involving vibronic couplings. In this work, the atomic structures of doped $LiCoO_2$ by Mg cation, F anion and both were investigated thoroughly to reveal the atomic environments of these dopants and their influence on the electrochemical performance. The function of these dopants is well addressed from the view of PJTE manipulation. Briefly, the $MgO_4$ tetrahedra in Mg-doped $LiCoO_2$ could suppress the charge transfer from ligand to Co in neighboring octahedra, thus depressing the PJTE. Although F doping does increase the ligand-field strength, the induced octahedral distortion reduces the structural stability dramatically. Comparatively, Mg/F co-doping generates the $CoO_5F$-$MgO_4F_2$-$CoO_5F$ medium-range orders (MROs), which could depress both structural distortion and charge transfer in Co-centered octahedra, significantly suppressing PJTE. The reduced PJTE accounts for the improved electrochemical performance, making the co-doped $LiCoO_2$ offers the best performance: a 70% capacity retention after 200 cycles within the potential range of 2.8-4.6 V, followed by Mg-doped $LiCoO_2$. In contrast, although F-doping could induce an extra rocksalt-like surface layer for higher capacity, its cycling improvement is rather limited. These results highlight the importance of structural modulation in enhancing the material performance, demonstrate that the manipulation of PJTE would be an effective strategy in developing novel high-performance oxide cathodes.

*Keywords: Li-ion batteries, Layered cathode, doping, electrochemistry.*

# Nanoporous $Li_4Ti_5O_{12}$ as anode material of Li-ion batteries for excellent high-rate performance

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## Abstract

Lithium titanate ($Li_4Ti_5O_{12}$, LTO) is used as an amazing anode material in Li-ion batteries, for several specific advantages associated with its unique spinel structure. For instance, there is no obvious volume expansion and contraction during lithiation/delithiation, enabling excellent cyclability and safety. In particular, the anode material could work in a wide temperature range from -50 ℃ to 70 ℃. However, the theoretical capacity of LTO is only 175 mAh/g, much less than that of graphite. To compensate the low capacity in practice, an excellent high-rate performance is necessary, and thus a nanoporous structure is very important because it facilitates the fast Li-ion diffusion.

Nanoporous spherical LTO was successfully prepared by spray drying method and the sequent calcination at 750 ℃. It is composed of many irregular polyhedra, and each irregular polyhedron has many polymerized nanocrystals, with a particle size of 20-35nm. At 1C rate, LTO electrode exhibited excellent electrochemical performance, characterized by a charging specific capacity of 170mAh/g and more than 99% retention after 100 cycles.

*Keywords: Li-ion batteries, Lithium titanate, Nanoporouis, electrochemistry.*

# Technical **Oral Session _ Session 7**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 7 (H7)** **10:50 - 12:20, Nov. 22**

**Chair :** To be announced 303B, 3F

10:50-11:10 **I-H0280** **[Invited] Giant converse magnetoelectric effect in Co2FeSi/PMN-PT multiferroic heterostructures**
Takamasa Usami (Osaka University, Japan)

11:10-11:30 **I-H0577** **[Invited] Multiscale structural parameters affecting antiferroelectric-ferroelectric phase transition**
Teng Lu (The Australian National University, Australia)

11:30-11:50 **I-H1078** **[Invited] Exotic phase transition mechanisms at ferroic multi-phase points**
Xiaoqin Ke (Xi'an Jiaotong University, China)

11:50-12:05 **O-H0900** **Sensitive magnetoelasticity by engineering nanoprecipitates**
Yiqun Zhang (Xi'an Jiaotong University, China)

12:05-12:20 **O-H0330** **Electrical resistivity and its temperature coefficient in Fe-Mn-Al-Cr-C-based alloys**
Nobuaki Takeuchi (Tohoku University, Japan)

# Giant converse magnetoelectric effect in $Co_2FeSi$/PMN-PT multiferroic heterostructures

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## Abstract

In multiferroic heterostructures consisting of ferromagnetic (FM)/piezoelectric layers, magnetism can be controlled by an electric field [1]. The feature is attractive for low-energy data writing in spintronic memory devices since conventional spintronic devices rely on the current-based control of magnetization direction with large energy consumption. To efficiently operate the heterostructure in practical devices, achieving the large converse magnetoelectric (CME) coefficient ($\alpha_E$) using a spintronic material is important. However, the multiferroic heterostructure using CoFeB known as a representative spintronic material shows $\alpha_E$ of ~$10^{-6}$ s/m [2], which is smaller than that of magnetostrictive materials with $\alpha_E$ of ~$10^{-5}$ s/m [3].

Among spintronic FM and piezoelectric materials, we have focused on multiferroic heterostructures composed of FM $Co_2$-Heusler alloys and $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN–PT) [4,5]. In this talk, we introduce the development of $Co_2$-Heusler alloy/PMN-PT heterostructures with the giant CME effect. Firstly, we describe the low-temperature growth of $Co_2FeSi$ on PMN-PT using the molecular-beam-epitaxy technique. Next, we show the experimental results demonstrating the giant $\alpha_E$ over $1\times10^{-5}$ s/m in $Co_2FeSi$/PMN-PT heterostructures [5].

This work was partly supported by JST CREST (Grant Number JPMJCR18J1), JSPS KAKENHI Grant (Numbers JP19H05616, JP20K21002, JP21K14196, and JP22H05000), and the Spintronics Research Network of Japan (Spin-RNJ).

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*Keywords: Multiferroic heterostructures, Magnetoelectric effect, $Co_2$-Heusler alloys, PMN-PT*

# Multiscale structural parameters affecting antiferroelectric-ferroelectric phase transition

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## Abstract

Polar functional materials, such as ferroelectrics (FEs), play a vital role in modern electronic devices like capacitors, sensors, and FeRAM. In addition to FE materials, antiferroelectric (AFE) materials with the antiparallel-aligned polar order have recently raised tremendous research interest due to their promising energy conversion and storage applications. These applications mainly stem from the unique structural transitions triggered by external stimuli like electric fields (E-field), temperature, and mechanical force. Consequently, it becomes pressing to unveil the structure parameters affecting the phase transitions. This study comprehensively investigates the structure-property relationship in the prototype $PbZrO_3$- and $AgNbO_3$-based antiferroelectric materials using complementary structural analytical techniques. It elaborates that structures at different lengths from the micro (domain alignment and crystallographic texture) to nano (correlated atomic displacements and octahedral tilting) scales impact the critical E-field required for triggering the AFE-FE phase transition. Moreover, it demonstrates that these critical structural parameters, which reflect the energy barrier between AFE and FE phases, can be modified through chemical compositions, external E-field, and temperature. The results illustrate that manipulating multiscale structure parameters allows for tuning AFE material properties. Importantly, these parameters can be adjusted not only through chemical compositions and synthesis conditions but also controlled by the history of applied E-field and temperature. Therefore, this study provides flexible structural parameters for tailoring the physical properties of AFE materials, offering new strategies to enhance the performance of AFE materials and devices.

*Keywords: Antiferroelectric, Phase transition, Neutron scattering, Diffuse scattering*

# Exotic phase transition mechanisms at ferroic multi-phase points

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**Abstract**

Ferroic multi-phase points, which include two-phase points, normally exhibit high sensitivity in response to external fields and thus attract much attention. The superior properties of ferroic multi-phase points relies on the phase transitions under external fields. Therefore, it is important to understand the phase transition mechanisms at ferroic multi-phase points. In recent years we have focused on the phase transition mechanisms at ferroic multi-phase points and made the following achievements: 1) Through synchrotron XRD experiments and phase field simulations, direct evidences of magnetization rotation mechanism at ferromagnetic two-phase points(morphotropic phase boundary) are provided for the first time, which are found to be due to the small magnetocrystalline anisotropy at the two-phase points; 2) A novel phase transition mechanism which is named as "polarization spinodal" mechanism is found to occur at ferroelectric two-phase points, which could help explain the high piezoelectricity at ferroelectric two-phase points; 3) Through Landau theory, it is found that a cubic-tetragonal-orthorhombic-rhombohedral four-phase point could exist at the temperature-composition phase diagram of a binary perovskite-structured ferroelectric systems and such four-phase points have to undergo a critical phase transition at Curie temperature. Due to the vanishing energy barrier at critical phase transitions, the four-phase points show large dielectric permittivity, large electrostrain and high flexoelectric coefficients. Our work unravels the exotic phase transition mechanisms at ferroic multi-phase points and it could shed light on the designing of high-sensitivity ferroic materials.

*Keywords: morphotropic phase boundary; ferroic multi-phase points; ferroic phase transition; phase rule*

# Sensitive magnetoelasticity by engineering nanoprecipitates

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## Abstract

Magnetoelasticity of materials refers to the capacity to convert magnetic energy into mechanical energy or vice versa, making them useful for sensors and energy harvesting. For most applications, it is desirable to have a combination of large magnetostriction and a small switching field, i.e. sensitive magnetoelasticity. However, simultaneously achieving large magnetostriction and small switching field is challenging because the magnetostriction and switching field are both proportional to the magnetocrystalline anisotropy (MCA). In this work, we shall present the achievement of sensitive magnetoelasticity by engineering nanoprecipitates. As exhibited in cubic alloy iron-gallium, coherent tetragonal nanoprecipitates formed at early-stage decomposition can simultaneously enhance the magnetostriction and reduce the switching field, giving rise to five-fold enhancement in the figure of merit, defined by saturation magnetostriction over MCA constant. The mutual elastic interactions between the coherent tetragonal nanoprecipitates and the soft matrix can result in an average tetragonal symmetry, i.e. substantially enlarge the saturation magnetostriction constant ($c/a$-1). The random magnetic interactions between the matrix and the dispersive nanoprecipitates can also result in the collapse of net MCA as well as the small switching field. By co-engineering the nanoprecipitates and grain orientations, the magnetoelasticity can be further enhanced. The feasibility of obtaining such two-phase nanostructure by aging a supersaturated solid solution then allows one to develop high-performance magnetostrictive materials from a large class of cubic ferromagnetic alloys.

*Keywords: Magnetoelasticity, Decomposition, Coherent nanoprecipitates, Magnetic anisotropy.*

**We wish to make presentation at Symposium H (Electronic and Magnetic Materials) in PRICM11.**

# Electrical resistivity and its temperature coefficient in Fe-Mn-Al-Cr-C-based alloys

**Nobuaki Takeuchi**[1], Masatoshi Iizuka[2], Daisuke Ando[3], Kiyohito Ishida[4], Yuji Sutou[5, 6]

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**Abstract (H: Electronic and Magnetic Materials)**

Improving the performance of resistors is essential for creating electronic devices that contribute to Society 5.0. Resistive materials used in resistors are required to have an appropriate electrical resistivity and a "low temperature coefficient of resistivity (TCR)," in which the resistivity hardly changes even when the temperature rises. Fe-Mn-Al-Cr-C alloys, known as high specific strength materials, have been found to combine high electrical resistivity with low TCR. However, the effect of heat treatment and structure on these properties is still unknown. In this study, we investigated the effect of heat treatment on these properties of Fe-Mn-Al-Cr-C alloy.

First, Fe-Mn-Al-Cr-C alloys were heat treated at 1100°C for 15 min followed by cold-rolling with a thickness reduction of 90%. And then, the obtained samples were heat treated in the temperature range of 200 to 1100°C. Electrical resistivity increased significantly with heat treatment above 500°C, but decreased with heat treatment above 900°C. These results were consistent with the variation of the α(BCC)/γ(FCC)-phase fraction, and the resistivity values were found to be proportional to the α/γ-phase fraction. The TCR decreased monotonically in the heat treatment temperature range above 600°C. However, although the α/γ-phase fraction of the samples was almost the same in the range of 600°C to 900°C, the TCR values differed greatly depending on the heat treatment temperature. The calculated phase diagram suggested that complex changes in the carbide phase fraction occurred in this temperature range, suggesting that the TCR value is greatly affected by the formation of carbide phases.

*Keywords: Fe-Mn-Al-Cr-C alloy, electrical resistivity, temperature coefficient of resistivity*

# Technical **Oral Session _ Session 7**

## **Symposium J :** Materials Characterization and in situ/3D/4D Analysis

**Materials Characterization and in situ/3D/4D Analysis 7 (J7)** **10:50 - 12:45, Nov. 22**

**Chair :** To be announced 201B, 2F

10:50-11:10 **I-J0538** **[Invited] Developing a New Set of Calibration Alloys for High-Temperature Thermal Analysis**
Kil-Won Moon (National Institute of Standards and Technology, USA)

11:10-11:25 **O-J0880** **Effects of crystallographic orientation on mechanical properties and deformation behaviours of small-volume copper**
HEQING LI (The University of Sydney, Australia)

11:25-11:40 **O-J0679** **In situ observation on the bonding of Al-Sn alloys to carbon steel**
Ahmad Zamanian Khorasgani (Pohang University of Science and Technology, Korea)

11:40-11:55 **O-J0767** **Investigation of mechanical behavior and serration deformation mechanism for structural materials at ultra-cryogenic temperature below 20K**
You Sub Kim (Chungnam National University, Korea)

11:55-12:10 **O-J0265** **Low temperature synthesis of high Sn concentration GeSn by electron beam irradiation**
Manabu ISHIMARU (Kyushu Institute of Technology, Japan)

12:10-12:25 **O-J0475** **Correlation of microstructure and the luminescence properties in GaN/InGaN multi-quantum wells grown on semi-polar m-plane sapphire substrate by using Transmission Electron Microscopy**
Young-Woon Kim (Seoul National University, Korea)

12:25-12:45 **I-J0769** **[Invited] Crystallographic mechanism of crack initiation and short crack growth during cyclic deformation in zirconium**
Conghui Zhang (Xi'an University of Architecture And Technology, China)

# Developing a New Set of Calibration Alloys for High-Temperature Thermal Analysis

Kil-Won Moon[1], Jiwon Park[2], Joohee Kang[3], Chang-Seok Oh[2], Carelyn Campbell[1], and Ursula Kattner[1]

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For accurate measurements of DSC/DTA at high temperatures (between 1100 °C to 1600 °C), a new set of binary eutectic alloys has been developed to serve as calibration standards. This set of alloys fills the temperature calibration gap between the melting points of Au (1064 °C) and Ni (1455 °C) and eliminates the significant uncertainty caused by the oxidation and vaporization of the pure Ni standard at the melting point. The candidate alloys also reduce the uncertainty from approximately ± 10 °C to less than ± 2 °C and enable the temperature calibration of commercial DSC/DTA within an interpolation range.

# Effects of crystallographic orientation on mechanical properties and deformation behaviours of small-volume copper

**Heqing Li**[1], Xianghai An[1]

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## Abstract

The plasticity of small-volume metals has been attracting dramatic attention as they serve as critical components to architect the micro/nano-electro-mechanical systems (M/NEMS). Extensive small-scale experimental and theoretical investigations revealed that the size-dependent plasticity is fundamentally dominated by the operation of dislocation sources, rather than the conventional dislocation interactions in their bulk counterparts. Previous studies also proposed that the formation of dislocation cells could be inhibited as the pillar size decreases to a critical value, resulting in improved strength and strain-hardening behaviour during the plastic deformation in Al. However, the underlying mechanisms pertinent to the absence of dislocation cells below the critical size remain unclear. Additionally, it is well-documented that crystallographic orientation plays a significant role in the activation of multiple slip systems, affecting the formation of the dislocation cells. Here we employ quantitative in-situ scanning electron microscope compression testings of single-crystal Cu pillars with diameters ranging from 500 nm to 5 μm to investigate the effects of sample sizes and orientations on the formation of dislocation cells and the consequent change of mechanical properties. Size and orientation-dependent work-hardening behaviour and deformation mechanisms were comprehensively explored, which were controlled by the interplay among sample size, crystalline orientation, and the formation of cell structures.

*Keywords: in-situ micropillar compression, crystallographic orientation effect, size effect, dislocation cells, strain-hardening.*

# In situ observation on the bonding of Al-Sn alloys to carbon steel

**Ahmad Zamanian Khorasgani[1],** Fazlollah Sadeghi[2], Tahereh Zargar[3], Yoon-Uk Heo[4], Jae-Sang Lee[5], Ho-Jae Kwak [6], Soo-Yeon Lee[7], Chang-Hee Yim[8]

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## Abstract

The Al–Sn alloys are considerably used as sliding bearing materials in combustion engines due to their excellent tribological and mechanical properties. Compared with the commercialized rolling technology, the casting method has more advantages due to its simplicity, however it is not commercialized yet because of different technological barriers including formation of strong bonding between clad material and steel substrate. In this study, real-time synchrotron X-ray in-situ observation is used to study the formation of the intermetallic compounds occurring at the interface of liquid clad Al-Sn alloy and solid carbon steel. Al-20 %wt. Sn and JIS S45C steel were fixed end to end and heated to different temperatures and subsequently cooled with different cooling rates to observe the morphology, formation mechanism and growth of inter-metallic compounds at the interface. The experimental findings indicate that upon heating and in the initial stages of melting, a layer of the tongue-like η phase (Fe2Al5) formed at the interface between of Al alloy and steel, and subsequently extended into the steel side. During the cooling phase prior to the initiation of solidification, the formation of the dotted θ-Fe4Al13 phase was observed. The occurrence of needle-like θ-Fe4Al13 phase near the interface or even within the Al-Sn alloy depends on the cooling rate and temperature conditions. Depending to the cooling rate and temperature, needle-like θ-Fe4Al13 phase also can be formed near interface or even in Al-Sn alloy. Moreover, the Sn phase distribute at θ-Fe4Al13 phase in very small size structure despite the near-network structure at the matrix grain boundary in Al alloy side.

*Keywords: Synchrotron Radiation X-ray, Interfacial bonding, Solidification, Al–Sn alloys, intermetallic compounds*

# Investigation of mechanical behavior and serration deformation mechanism for structural materials at ultra-cryogenic temperature below 20K

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**Abstract**

Liquid hydrogen energy has attracted much attention as next-generation green energy to achieve carbon neutrality because liquid hydrogen has high energy density and eco-friendly than other energy source. In order to transport and store liquid hydrogen, structural metallic materials will primarily be used. However, these materials can only be used at ultra-cryogenic temperature below 20K. Since the mechanical properties and deformation mechanisms of metallic materials are highly dependent on temperature, it can be challenging to predict how much the mechanical properties deteriorate and what kinds of deformation mechanisms are driven at extreme low temperature. Although studies on the mechanical properties of metallic materials at 77K have been widely reported, few research papers have evaluated their physical properties under 20K. Especially, it is known that a new deformation mechanism called as serration deformation is occurred at ultra-cryogenic temperature. To shed light on this, we conducted in-depth study of the mechanical behavior and serration deformation mechanism at ultra-cryogenic temperature via in-situ neutron diffraction and metallurgical analysis. In-situ neutron diffraction experiments were performed to study the tensile behavior of structural materials under 20K. The entire diffraction patterns monitored during tensile loading enabled us to examine evolution of 1) lattice strains by diffraction peak shift, 2) phase transformation by peak generation, and 3) localized microstructure by diffraction peak broadening. In particular, macroscopic stress-strain response, microscopic elastic-plastic deformation, and strain hardening behavior during tensile loading were compared at room temperature and ultra-cryogenic temperature.

*Keywords: Ultra-cryogenic temperature, In-situ neutron diffraction, Mechanical properties, Serration deformation, Peak profile analysis*

# Low temperature synthesis of high Sn concentration GeSn by electron beam irradiation

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## Abstract

Fabrication of group-IV semiconductor thin film transistors on plastic substrates is of technological importance for realizing high-performance flexible electronics. Recrystallization of amorphous is one of the possible ways to produce polycrystalline semiconductor films, and therefore much effort has been devoted to reduce the crystallization temperature. Because adding Sn to Ge can lower the recrystallization temperature and increase the carrier mobility, GeSn is attracting attention as a thin-film transistor for next-generation flexible displays. However, the solubility limit of Sn in crystalline Ge is ~1.1 at% at 400 ºC, and Sn segregation easily occurs during thermal annealing.

Radiation-assisted materials synthesis can achieve atomic arrangements far from equilibrium state through non-thermal processes. We have found that electron-beam-irradiation can induce the recrystallization of amorphous materials at room temperature, and therefore this technique is useful for establishing the low temperature synthesis of GeSn polycrystalline thin films. To establish the low temperature processing, knowledge of crystallization processes is required. In the present study, the crystallization processes of amorphous GeSn under low-energy electron-beam irradiation were examined using transmission electron microscopy (TEM). The following results were obtained: (1) Electron-beam irradiation can induce the crystallization of amorphous GeSn via electron excitation effects. The resultant crystalline GeSn includes ~30 at.%Sn; (2) The temperature rise during electron irradiation was estimated to be less than 20 K, and low-temperature synthesis of crystalline GeSn can be realized by electron-beam irradiation; (3) *In situ* TEM observations revealed that rapid liquid-mediated crystallization results in the formation of large grains on the order of micrometers.

*Keywords: Radiation effects, amorphous, crystallization, transmission electron microscopy*

# Correlation of microstructure and the luminescence properties in GaN/InGaN multi-quantum wells grown on semi-polar *m*-plane sapphire substrate by using Transmission Electron Microscopy

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## Abstract

GaN/InGaN multi-quantum well (MQW) thin films were grown on the semi-polar (11-22) GaN to improve the luminescence efficiency by minimizing the piezo-electric effect. Three types of BSFs: $I_1$, $I_2$, and $E$, which are commonly reported defects in wurtzite GaN [1] are known to be difficult to identify because it is hard to distinguish using $\boldsymbol{g \cdot R}$ invisibility [2]. In this study, we applied cathodoluminescence in transmission electron microscopy (TEM-CL), which clearly identifies the types of BSFs and visualizes their distribution at a glance, with a high spatial resolution. $I_1$-BSF type defects spread throughout the film with high number density while the $I_2$-BSF type defect exists as a form of thin strips with less population. PDs and BSF-related defects existed in the form of short-segmented lines but with strong luminescence characteristics. Optical fingerprint identification of crystallographic defects based on TEM-CL can be applied to investigate the emission characteristics originating from defects in various growth.

[ 1] Drum C. 1965 *Phil. Mag.* **11** 313-334
[ 2] Dasilva Y. A., *et al.* 2010 *J. Phys.: Cond. Matter* **22** 355802

*Keywords: Cathodoluminescence, Transmission Electron Microscopy, GaN/InGaN multi-quantum well, semi-polar GaN, m-plane sapphire, Indium concentration.*

# Crystallographic mechanism of crack initiation and short crack growth during cyclic deformation in zirconium

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**Abstract**

Fully-reversed cyclic deformation of a pure Zr was conducted at strain amplitudes of 0.4% and 0.8% to investigate the deformation and crack initiation behaviors based on slip trace analysis. It was found that prismatic <a> slip with higher Schmid Factor ($m$ >0.4) was the dominant deformation mode. The grains containing persistent slip bands (PSBs) tended to go towards $[\bar{1}2\bar{1}0]$ pole, and the Schmid Factor (SF) had a critical value of 0.4 above which prismatic and pyramidal slip were dominant. Fatigue cracks were mainly initiated at PSBs and grain boundaries (GBs). It showed that the percent of PSB cracks were 61.1% and 53.5% under strain amplitude of 0.4% and 0.8%, respectively. PSB cracks were mainly parallel to prismatic <a> slip with higher SF while some cracks tended to be initiated at GBs with higher misorientation angles. Short fatigue crack growth (SFCG) behavior of zirconium was quantitatively investigated. Results show that the SFCG was mainly transgranular, sensitive to crystallographic orientation which determined the slip systems within grains and often deflected at GBs. The cracks propagated preferentially on prismatic and pyramidal slip planes due to higher SF for each grain. A set of crack deflection at GBs was quantitatively analyzed. A combination of the geometrical compatibility factor, $m'$, and twist angle, $\alpha$, as well as the Schmid factor, $m$, were proposed to evaluate SFCG across grain boundaries. It was found the SFCG could cross GBs on the conditions of $m > 0.3$, $\alpha < 40^{\circ}$, and $m' > 0.3$.

*Keywords: Fatigue crack initiation; Short fatigue crack growth; Grain boundary; persistent slip bands; crystallographic orientation.*

# Technical **Oral Session _ Session 7**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 7 (K7)** **10:50 - 12:25, Nov. 22**

**Chair :** Karam Lim (Korea Institute of Materials Science) Samda Hall B, 3F

10:50-11:20 **K-K0576** **[Keynote] Strategy for tailoring thermoplastic forming process in bulk metallic glasses**
Eun Soo Park (Seoul National University, Korea)

11:20-11:40 **I-K0188** **[Invited] Effect of quenched strain on the rejuvenation of ferromagnetic amorphous ribbons**
Masato Ohnuma (Hokkaido University, Japan)

11:40-11:55 **O-K1101** **Phase-selective recrystallization makes eutectic high-entropy alloys ultra-ductile**
Qingfeng Wu (Pohang University of Science and Technology, Korea)

11:55-12:10 **O-K0321** **Amorphization of Si in Al88Si12 eutectic alloy with liquid quenching**
Rui Yamada (Tohoku University, Japan)

12:10-12:25 **O-K0376** **Cluster-model-based composition genes for high-entropy alloys and metallic glasses**
Shuang ZHANG (Dalian Jiaotong University, China)

# Strategy for tailoring thermoplastic forming process in bulk metallic glasses

Wook Ha Ryu[1], Min Kyung Kwak[2], Chae Woo Ryu[3], Hyunseok Oh[4], **Eun Soo Park[5]**

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## Abstract

The technical interest in bulk metallic glasses (BMGs) has grown over the past few decades due to their potential for new areas of applications based on thermoplastic forming (TPF), which was previously unattainable in conventional crystalline alloys. However, the difficulty in controlling the TPF process due to the metastability of the amorphous phase has posed a barrier to widespread commercial use. This study provides practical guidelines for tailoring the TPF process, incorporating the influence of process variables in BMGs. Specifically, first, a practical indicator of the ideal thermoplastic forming ability (TPFA) of metallic glasses ($\Delta T_F = T_l - T_x$) is proposed by comprehensively considering flow instability and phase stability. Using this indicator, it is possible to easily select superior glass-forming alloy systems with excellent TPFA. Secondly, we accurately identify the TPF window and TPFA according to the heating rate in a wide range from $10^{-1}$ to $10^4$ K/s, based on constructing the continuous heating transform (CHT) diagram with iso-viscosity contours. These approaches enable the selection of customized TPF processes for each amorphous alloy, providing guidelines for the selection of tailored TPF processes. Finally, as an example of a TPF process, we demonstrated three TPF procedures from bulk to nano scales, namely BMG pressing, BMG joining, and hologram nanopatterning in LM1b ($Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$) utilizing the obtained CHT diagram. These results will enable us to select the most suitable BMG for targeted applications and precisely optimize the TPF processes, which could lead to further improvements in their performance and expanded applications in various industries.

*Keywords: Bulk metallic glass; Thermoplastic forming; Thermoplastic formability parameter; Continuous heating transformation curve; Processing optimization*

# Effect of quenched strain on the rejuvenation of ferromagnetic amorphous ribbons

**Tomoya Oshikiri[1], Masato Ohnuma[1], Junji Saida[2], Rui Yamada[3], Motoki Ohta[4]**

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## Abstract

Fe, Ni, Co-based metallic glasses are now commonly used in electronic coils, transformer etc. They are ferromagnetic ribbons and show excellent magnetic softness. Most of the ribbons are used after a certain heat treatment, some for releasing strain and the others for giving a strain for obtaining uni-axial magnetic anisotropy. We have recently found that the elastic strain is quenched by annealing under stress and they release it by heating to the same temperatures with that of previous stress annealing [1,2]. Through these studies, we can now control the residual strain level. Using this effect, we discuss the effect of rejuvenation treatment which include cyclic heat treatments by dipping to warm water and $LN_2$ several times. We prepare three alloys with different strain level, i.e. as-quenched, pre-heated for releasing residual strain and rolled Fe-Si-B metallic glass and evaluate newly introduced strain by rejuvenation treatment. The results show clear difference of the strain level; the effect is the smallest in the pre-heated ribbons and the largest in the rolled ribbon. The relationship between quenched strain and thermal strain introduced by rejuvenation treatment is not straightforward in regular alloys. However, the relation can be strong in the alloy with invar effect. Fe-Si-B shows strong invar effect, therefore, we compare the rejuvenation effect to that of CoFe-Mn-Si-B metallic glass which does not show the invar effect. The results will be shown in the talk.

[1] Kozikowskiet al., Scripta Mater. **67**, 763 (2012).
[2] Kozikowskiet al., Physical Review Materials, 4(2020), #095604

*Keywords: quenched strain, rejuvenation, ferromagnetic metallic glass ribbons*

# Phase-selective recrystallization makes eutectic high-entropy alloys ultra-ductile

**Qingfeng Wu[1,2],** Feng He[1], Junjie Li[1], Hyoung Seop Kim[2*], Zhijun Wang[1*], Jincheng Wang[1*]

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**Abstract:**

Excellent ductility is crucial not only for shaping but also for strengthening metals and alloys. The ever most widely used eutectic alloys are suffering from the limited ductility and losing competitiveness among advanced structural materials. Here we report a distinctive concept of phase-selective recrystallization to overcome this challenge for eutectic alloys by triggering the strain hardening capacity of the duplex phases completely. We manipulate the strain partitioning behavior of the two phases in a eutectic high-entropy alloy (EHEA) to obtain the phase-selectively recrystallized microstructure with a fully recrystallized soft phase embedded in the skeleton of a hard phase. The resulting microstructure fully releases the strain hardening capacity in EHEA by eliminating the weak boundaries. Our phase-selectively recrystallized EHEA achieves a high ductility of ~35% uniform elongation with true stress of ~2 GPa. This concept is universal for various duplex alloys with soft and hard phases and opens new frontiers for traditional eutectic alloys as high-strength metallic materials.

**Keywords:** eutectic high-entropy alloy, recrystallization, strain partitioning, deformation mechanism

# Amorphization of Si in $Al_{88}Si_{12}$ eutectic alloy with liquid quenching

**Rui Yamada[1],** Junpei. T. Okada[1], Takeshi Wada[1], Junji Saida[2], Hidemi Kato[1]

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**Abstract**

An amorphous Si is one of the important materials for many engineering applications. Recently, our collaborative research group of Okada et al. found a presence of an amorphous state of Si together with a crystalline Al in a $Al_{88}Si_{12}$ binary eutectic ribbon sample prepared with a melt spinning technique[1)]. So far, it has been thought to be difficult to obtain an amorphous state of Si from a liquid by using a single pure Si element as a starting material. However, we clearly revealed that using Al-Si alloys made it possible to produce the amorphous state of Si from liquids. Currently, two factors, i) a large extent of supercooling and ii) created peculiar solidified microstructures seem to be keys for achieving amorphization of Si, though the details are still uncertain. In a present study, $Al_{88}Si_{12}$ liquid quenched samples with different cooling rates were firstly prepared and then, their amorphous natures and solidified microstructures were thoroughly investigated. By applying a coupled zone concept[2)], we successfully explained the created solidified microstructures with different cooling rates, which will lead to an elucidation of the amorphization mechanism of Si from a liquid.

1) J. T. Okada, K. Nakayama, T. Wada, R. Yamada et al., submitted.
2) W. Kurz, D. J. Fisher, International Metals Reviews 24, 1979, 177-204.

*Keywords: Amorphization of silicon, binary eutectic alloy, liquid quenching, coupled zone*

# Cluster-model-based composition genes for high-entropy alloys and metallic glasses

**Shuang Zhang[1]**, Chuang Dong[1,2], Cunlei Zou[1], Yajun Zhao[1]

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## Abstract

High-performance materials always possess specific chemical compositions, which strongly suggest the possible existence of some molecule-like structural units, in which the versatile but specific compositions are rooted. These structural units mimic the molecules in chemical substances but generally differ from the crystallographic unit cells. The possibility of having these fundamental units has been apparently overlooked because of the lack of structural models to properly address the short-range orders in materials. Our research group has already proposed the cluster-plus-glue-atom model in 2007, which is a short-range-order structural model that renders any structure with a structural unit containing the essential structural information of the whole system. From the nomination of this model, one immediately determines a molecule-like structural unit consisting of a nearest-neighbor cluster plus a few outer-shell glue atoms. Actually, such structural unit, serving as the composition carrier, can be seen as the composition gene of the material.

In the present work, Friedel oscillations, in combination with the cluster-plus-glue-atom model, are fully presented to show how to uncover the composition genes hidden in chemical short-range orders in any material. Examples are then given in various high-entropy alloys and metallic glasses, including Al-Cr-Fe-Co-Ni high-entropy alloys, stainless steels with high-entropy alloying feature, Cu-Zr bulk metallic glasses, $Zr_{55}Cu_{30}Al_{10}Ni_5$ multi-component bulk metallic glass, etc. The proposition of composition genes supports a new perspective for the research of high-entropy alloys and metallic glasses, facilitates the understanding of prevailing materials, and can be a useful tool to guide the exploration of new composition space.

*Keywords: Cluster-plus-glue-atom model; Molecule-like structural units; Composition genes; High-entropy alloys; Metallic glasses*

# Technical **Oral Session _ Session 7**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 7 (L7)** **10:50 -12:30, Nov. 22**

**Chair :** Elizabeth Kyriakou L (University of Technology Sydney), Soo-Hyun Joo (Dankook University) **202B, 2F**

10:50-11:20 **K-L0247** **[Keynote] Biofunctionalization of Titanium by Surface Treatments**
Takao Hanawa (Tokyo Medical and Dental University, Japan)

11:20-11:40 **I-L0104** **[Invited] Microstructure and specific properties of heterogeneous-nanostructured stainless steel and copper alloys fabricated by heavy cold rolling**
Hiromi Miura (Toyohashi University of Technology, Japan)

11:40-12:00 **I-L0661** **[Invited] Formation of an onion-like two-phase structure in refractory-metal based alloys**
Seiji Miura (Hokkaido University, Japan)

12:00-12:15 **O-L0055** **Effect of quenching temperature on microstructure and properties of a stainless clad steel plate 316L/Q500 for bridge structure**
Fan Zhen (Shagang Group, China)

12:15-12:30 **O-L0137** **Deformation behavior of heavily cold-rolled duplex stainless steel with and without aging**
Chihiro WATANABE (Kanazwa University, Japan)

# Biofunctionalization of Titanium by Surface Treatments

**Takao Hanawa**[1,2,3]

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## Abstract

Approximately 80% of implant medical devices are made of metal, and metals therefore continue to play an important role in medical treatment. Current research efforts in metallic biomaterials are made with the following categories: the elucidation of interfacial reactions between metals and tissues (including evaluations of safety and corrosion resistance); the development of new surface treatment techniques (including the control of surface morphology); the development of new alloys; and the development of new manufacturing processes. In particular, surface treatment is an important tool to add biocompatibility and biofunction to metals. Target surface finishing by surface treatments is categorized in the lecture. To achieve a dual-functional surface both with bone formation and antibacterial properties, a sufficient quantity of Ag, Cu, and Zn are added into the electrolyte for micro-arc oxidation (MAO). An effective concentration of Ag, Cu, and Zn for the dual function is appeared: In this concentration region, both the osteogenesis and antibacterial activity appears. On the other hand, to clarify the effects of micron/nano-meter level topography on cell behavior and morphology, we investigated the adhesion of human mesenchymal stem cell (hMSC) to Ti surfaces with micron/nano grooves and grids which created using a femtosecond laser. The different surface features had different effects on the differentiation of hMSC. Metal surface is possibly biofunctionalized by various surface modification techniques. These techniques make it possible to apply metals to a scaffold in tissue engineering and regenerative medicine.

*Keywords: Metallic biomaterial; surface treatment; biofunction; biocompatibility.*

# Microstructure and specific properties of heterogeneous-nanostructured stainless steel and copper alloys fabricated by heavy cold rolling

**Hiromi Miura[1],** Yoshiteru Aoyagi[2], Yojiro Oba[1], Masakazu Kobayashi[1], Chihiro Watanabe[3]

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## Abstract

SUS316LN austenitic stainless steel and Cu-Zn system alloys were heavily cold rolled to 92% in reduction at maximum to develop heterogeneous nanostructure comprising “eye”-shaped twin domains, shear bands and conventional low-angle lamellae. The grain-boundary spacings in the twin domains and the low-angle lamellae were about 25 nm and 40 nm in average, respectively. The twin domains were surrounded by shear bands with an average width of about 40 nm and embedded in the low-angle lamellae. It showed large anisotropy of mechanical properties that the tensile strength along transverse direction, 1.9 GPa, was much higher than that along rolling direction, 1.6 GPa for SUS316. Although quite high tensile strength was achieved, ductility was not largely spoiled. The superior mechanical properties and the anisotropy could be understood from the distribution of the heterogeneous-nanostructure components and crystallographical orientations. The tensile strength was further raised by aging up to 2.2 GPa and 1.9 GPa, respectively. heterogeneous nanostructured Cu-Zn alloys also exhibited superior mechanical properties as well as electroconductivity. It was found that segregation of solute elements at twin and low-angle lamellar boundaries, which were major structural components, induced additional strengthening by aging. It was concluded, therefore, that combined strengthening mechanisms of grain refinement by the evolution of nano-lamellar structures and grain-boundary segregation caused excellent mechanical properties.

*Keywords: Heterogeneous nanostructure, Mechanical twin, Strength, Microstructure, grain boundary segregation*

# Formation of an onion-like two-phase structure in refractory-metal based alloys

**Seiji Miura**[1], Hayato Himukai[2], Syuki Yamanaka[3], Ken-ichi Ikeda[4], Satoshi Takizawa[5], Seiichi Watanabe[6]

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## Abstract

It is newly found that an onion-like two-phase structure is formed in refractory-metal based alloys composed of Nb, Ta and Zr during a heat-treatment for spinodal decomposition. A 3D multi-shell-structure is confirmed by SEM-FIB observation. SEM-EBSD observation revealed each of shell are single phase. 3D phase-field simulation revealed that the onion structure is initiated at an edge of concentration profile which might be introduced during solidification as dendrites. The mechanical properties and cracking behavior investigated by using Vickers indentation will be discussed.

*Keywords: Spinodal decomposition, multi-shell structure*

# Effect of quenching temperature on microstructure and properties of a stainless clad steel plate 316L/Q500 for bridge structure

**Fan Zhen[1],** ChunJuan Shao[1], Jinbo Qu[1], Han Ma[1], Jing Liu[2], Feng Huang[2], Xiaobing Li[3]

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## Abstract

Stainless clad steel plate is a composite steel plate made by bonding stainless steel plate (cladding material) to either or both sides of a carbon steel plate (base metal). Featuring not only sufficient strength but good corrosion resistance, stainless clad steel plate has been used in a variety of industrial applications including shipbuilding, pressure vessels and bridge structures. One of the key mechanical measures of stainless clad steel plate is the interfacial bonding strength between stainless and carbon steel plates, which is mainly governed by hot rolling and heat treatment process.

In this study, a 500MPa high strength grade stainless clad steel plate, 316L/Q500 for bridge structure, was investigated with an emphasis on the effect of quenching temperature. Different quenching temperatures ($T_Q$), ranging from 850 to 1050°C, was conducted on the test plate and the interfacial characteristics, i.e. carburized and decarburized layer depths and bonding strength, were measured. It was observed that with the increase of $T_Q$, the depths of carburized layer (CL) and decarburized layer (DL) decreased, and became zero when $T_Q$ reached 1050°C and 900°C, respectively. The interfacial bonding strength was found increased first and then decreased with the increase of $T_Q$. In addition, the variation of strength with $T_Q$ was also tested on 316L and Q500 separately. The result showed that the yield and tensile strengths of 316L decreased, while that of Q500 increased as $T_Q$ increased. When $T_Q$ was above 900°C, the calculated strengths based on the rule-of-mixtures was greater than the measured ones.

*Keywords: Stainless clad steel plate; 316L/Q500; Quenching temperature; Interfacial bonding strength; Rule of mixtures*

# Deformation behavior of heavily cold-rolled duplex stainless steel with and without aging

**Chihiro Watanabe[1],** Koga Norimitsu[2], Yoji Miyajima[3], Hiromi Miura[4]

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## Abstract

The deformation behavior of heavily cold-rolled ferrite-austenite duplex stainless steel with or without aging was systematically investigated. Evolution of the typical heterogeneous-nano (HN) structure was confirmed in the austenite (γ) phase after heavy cold rolling, whereas classical substructure was simply formed in the ferrite (α) phase. Aging at 723 K increased both yield stress and ultimate tensile strength (UTS) of the duplex stainless steel, while aging at 773 K increased only the UTS. Nanoindentation hardness tests were performed on the specimens before and after aging. The γ phase had a higher hardness than the α one in the as-rolled specimen. Peak aging at 723 K resulted in a significant increase in hardness in both phases. On the other hand, aging at 773K hardly changed the hardness of the α phase while it of the γ one increased slightly. In-situ X-ray measurements were performed to examine the variation of the phase stress during deformation. After macroscopic yielding, a remarkable stress partitioning from the α to the γ phase occurred. Age hardening at 723 K of the α phase effectively contributed to the increase in the yield stress and UTS. In contrast, an increase in ductility due to recovery of the α phase during aging at 773 K resulted in higher phase stress in the γ one, thus achieving lower yield stress but higher UTS. Therefore, it can be concluded that age hardening of the α phase is particularly important for the overall strengthening of the HN-structured duplex stainless steel.

*Keywords: Duplex stainless steel, heterogeneous-nano structure, aging, phase stress, stress partitioning*

# Technical **Oral Session _ Session 7**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 7 (M7)** **10:50 - 12:30, Nov. 22**

**Chair :** Lei Lu (CAS), Yakai Zhao (A*STAR) 402, 4F

10:50-11:20 **K-M0165** **[Keynote] Strengthening of pure Ti by severe plastic deformation: use of grain refinement and allotropic transformation**
Zenji Horita (Saga University, Japan)

11:20-11:40 **I-M1090** **[Invited] Alkaline carbonate as high temperature lubricant for hot metal forming**
Long Wang (Northwestern Polytechnical University, China)

11:40-12:00 **I-M1106** **[Invited] An ultrafine-grained cost-effective medium entropy alloy with promising mechanical and tribological properties: Development and potential applications**
Guanyu Deng (The University of Queensland, Australia)

12:00-12:15 **O-M0318** **Impact of high-pressure torsion on crystal structural and functional properties of Si and Ge**
Yoshifumi Ikoma (Kyushu University, Japan)

12:15-12:30 **O-M0320** **Fabrication of Rocksalt Structure of ZnO using Severe Plastic Deformation under High Pressure**
Yongpeng Tang (Kyushu University, Japan)

# Strengthening of pure Ti by severe plastic deformation: use of grain refinement and allotropic transformation

**Zenji Horita**[1,2,3]

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## Abstract

According to the temperature-pressure phase diagram of pure Ti [1], allotropic transformation occurs from α phase with an hcp crystal structure to ω phase with a simple hexagonal crystal structure upon application of pressures at ambient temperature. Nevertheless, the ω phase remains present even after removal of the pressure when pure Ti is severely deformed under high pressure as by high-pressure torsion (HPT) [2]. Because the hardness is higher in the ω phase than the α phase and significant grain refinement is achieved by the HPT process, it may be possible to anticipate high-strength Ti without addition of alloying elements such as Al, V and Mo. However, the ω phase appears to be brittle [2] and it is not appropriate for simple mixtures of the two phases but the ω phase should be finely dispersed in the ductile α matrix as in the conventional dispersion strengthening materials. This presentation introduces our recent challenging for fabrication of a fine dispersion of the ω phase in the ultrafine-grained α matrix to increase the strength with reasonable ductility.

The structural change of pure Ti processed by HPT during post-annealing was observed by *in-situ* X-ray diffraction analysis using BL04B1 of SPring-8 [3]. Tensile tests were conducted not only on the HPT-processed samples but also subsequently heat-treated samples.

[1] R. G. Hennig *et al.*: Nature Mater. **4** (2005) 129-133.
[2] K. Edalati *et al.*: Metall. Mater. Trans. A **40** (2009) 2079-2086.
[3] Z. Horita *et al.*: Mater. Trans. **62** (2021) 167-176.

*Keywords: Severe plastic deformation, high-pressure torsion, pure titanium, phase transformation, X-ray diffraction analysis*

# Alkaline carbonate as high temperature lubricant for hot metal forming

**Long Wang**[1], Weimin Liu[1]

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## Abstract

Many industrial processing operations involve hot metal forming. In the rubbing counterparts of the interacting surfaces at high temperature, lubrication is crucial in reducing friction and wear for the hot metal forming process, the benefits include a reduced energy consumption, a reduced tool/component wear and a longevity of moving machine parts. Graphite based lubricants has been widely used. However, energy and environment concern require new and "white" lubricant to replace the conventional graphite or oil contained lubricant. At high temperatures and under high shear conditions, some inorganics transition from the solid into a semi-liquid phase (melt) can occur, which can lubricate the sliding interface.

Alkaline carbonate is a water-soluble environmental-friendly salt, which has a wide range of applications in glass manufacturing, food additives, cooking etc. They melt in the temperature range from 750-890 °C, which is likely to offer lubrication for the hot metal forming. This work reports the potential application of alkaline carbonate as an environmentally friendly and inexpensive high-temperature lubricant for hot metal rolling of steel. Its performance was evaluated by the ball-on-disc tribo-tests at high-temperatures. Significant reduction of friction and wear was achieved, which was attributed to the tribo-induced melting of sodium carbonate at the sliding interface, which acted as a liquid lubrication layer and formed a shear-induced nano-gradient tribofilm structure. The sodium carbonate melt was readily sheared and produced low friction and negligible wear. The nano-gradient tribofilm structure which formed under sliding inhibits cracking and spalling, resulted in a low wear due to strain delocalization.

*Keywords:* Hot metal forming, Lubricant, Nano-gradient tribofilm, Alkaline carbonate, Tribology

# An ultrafine-grained cost-effective medium entropy alloy with promising mechanical and tribological properties: Development and potential applications

**Guanyu Deng[1]**, Yu Yin[1], Huijun Li[2], Ming-Xing Zhang[1]

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## Abstract

High entropy alloys (HEAs), as a new class of metallic materials, have attracted considerable interest in recent years owing to their outstanding properties. However, the practical application of HEAs is significantly restricted by its high cost, which thus promotes the development of novel low cost HEAs without expensive elements or medium entropy alloys (MEAs) containing less principle elements. In the present study, a Co-free MEA with ultrafine-grained microstructure has been specifically produced by conventional thermal-mechanical processing method. It has been found that the ultrafine-grained MEA exhibits excellent mechanical properties, high corrosion resistance, as well as promising tribological performance in a wide temperature range. The outcome of this research demonstrates a great potential application of this cost-effective MEA for extreme conditions.

*Keywords: Medium entropy alloy; Ultrafine-grained microstructure; Mechanical properties; Corrosion resistance; high-temperature wear properties.*

Photo of the Invited Speaker



# Impact of high-pressure torsion on crystal structural and functional properties of Si and Ge

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## Abstract

Group-IV elements Si and Ge are the major semiconductor materials for modern electronic devices. However, the indirect bandgaps of Si (1.12 eV) and Ge (0.66 eV) hinder the widespread application of semiconductor devices. The application of severe plastic deformation is promising because the physical properties of Si and Ge can be altered by grain refinement and the formation of metastable phases. We have applied high-pressure torsion (HPT) to Si and Ge at a nominal pressure of 24 GPa, and found the formation of metastable phases such as Si-III (bc8), Si-XII (r8), and Ge-III (st12) as well as the formation of nanograins. However, the effect of shear strain during HPT processing at lower pressures (< 10 GPa) on the structural and functional properties has not been fully understood. In this study, we investigated the HPT processing of Si and Ge at the nominal pressure of 6 GPa. The HPT-processed Si and Ge samples consisted of Si-III/XII and Si-I, and Ge-III and Ge-I, respectively. The resistivity of Si increased after HPT processing for 10 anvil rotations ($N$), and it decreased when $N \geq 50$. The resistivity of Ge increased with increasing $N$. These results indicate that the strain-induced phase transformation from Si-I/Ge-I to high-pressure Si-II/Ge-II occurred during HPT processing at 6 GPa, and semimetallic Si-III and semiconductor Ge-III were formed upon unloading.

*Keywords: severe plastic deformation, high-pressure torsion, Si, Ge, metastable phase*

# Fabrication of Rocksalt Structure of ZnO using Severe Plastic Deformation under High Pressure

**Yongpeng Tang**[1], Kaveh Edalati[2], Takahiro Masuda[3], Yuji Higo[4], Satoshi Iikubo[1], Zenji Horita[5,6,7]

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## Abstract

Zinc oxide (ZnO), possessing a rocksalt crystal structure, is attractive because of the bandgap which lies within the range of visible light absorption (1.2-2.6 eV). However, the rocksalt structure is not stable at ambient pressure and temperature according to an equilibrium phase diagram. In this study, ZnO powder is initially processed by high-pressure torsion (HPT). The HPT-processed ZnO is then examined using a high-pressure application system available at BL04B1 of SPring-8 and in situ X-ray diffraction (XRD) analysis is conducted under high pressures at elevated temperatures. As a result, a 100% fraction of the rocksalt structure is obtained at ambient pressure and temperature. The results indicate that the initial presence of the rocksalt structure produced by the HPT process is effective to attain a 100% fraction of the rocksalt structure.

*Keywords: severe plastic deformation, high-pressure torsion, ZnO, rocksalt structure, wurtzite structure*

# Technical **Oral Session _ Session 7**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 7 (N7)** **10:50 - 12:35, Nov. 22**

**Chair :** Kunok Chang (Kyung Hee University) 203, 2F

10:50-11:20 **K-N0869** **[Keynote] Accelerating the Discovery and Design of Novel Materials by ALKEMIE**
Zhimei Sun (Beihang University, China)

11:20-11:40 **I-N0238** **[Invited] Precipitates in Al-Cu-Li alloys: First-principles and Experimental study**
Kyoungdoc Kim (Pohang University of Science and Technology, Korea)

11:40-12:00 **I-N0179** **[Invited] High-accuracy prediction of dendritic solidification microstructure through GPUs and AMR-accelerated computation**
Shinji SAKANE (Kyoto Institute of Technology, Japan)

12:00-12:20 **I-N1018** **[Invited] Augmented Phase-field Model with Finite Interface Dissipation**
Lijun Zhang (Central South University, China)

12:20-12:35 **O-N0830** **Super resolution of three-dimensional microstructural image of a steel using deep learning**
Hoheok Kim (Korea Institute of Materials Science, Korea)

# Accelerating the Discovery and Design of Novel Materials by ALKEMIE

**Zhimei Sun**

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**Abstract**

The development of high-throughput automation integrated-computations and data mining algorithms based on material databases and artificial intelligence algorithms is crucial for accelerating the discovery and design of novel materials. In this talk, I will present an open-source distributed computational platform named Artificial Learning and Knowledge Enhanced Materials Informatics Engineering (ALKEMIE) which is based on the AMDIV (automation-modular-database-intelligence-visualization) design concepts. Additionally, I will also present ALKEMIE-MatterDB, which contains multi-type materials database of structure, task, workflow and material property. Combining with the power of supercomputing, ALKEMIE enables the rapid deployment of artificial intelligence algorithms in the design of new materials. Finally, some examples of the discovery and design of novel materials using ALKEMIE will be demonstrated.

*Keywords: ALKEMIE, high-throughput calculations, artificial intelligence algorithm*

# Precipitates in Al-Cu-Li alloys: First-principles and Experimental study

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## Abstract

In this presentation, we provide an overview of thermodynamic stability of T1 phase in Al-Cu-Li alloys. We recently investigated the bulk and interfacial thermodynamic stability of T1 phase using a first-principles density-functional theory calculations. We find that the DFT-predicted T1 phase at 0K has two-different stoichiometry of Al6Cu4Li3 and Al13Cu7Li6. We also derive a low-energy T1/Al coherent interfacial structure and find that Ag and Mg solutes are predicted to segregate to the coherent interface, which agrees with recent experimental observations by atom probe tomography. This work will shed light on the multi-scale modeling of T1 precipitates, ultimately, designing high-performance of Al-Cu-Li alloys using the Integrated Computational Materials Engineering (ICME).

*Keywords: Aluminium Alloys, First-principles Calculation, Density-Functional Theory*

# High-accuracy prediction of dendritic solidification microstructure through GPUs and AMR-accelerated computation

**Shinji Sakane**[1], Takayuki Aoki[2], Tomohiro Takaki[3]

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## Abstract

Mechanical properties of products manufactured by casting, welding, and additive manufacturing are determined by solidification microstructure of those products which pose industrial challenges in their accurate prediction. Dendrite growth, a typical formation process of solidification microstructure, is a complex multi-physics phenomenon involving solid–liquid phase transformation, heat and solute transfer, melt convection, and solid transport. The phase-field (PF) method has been developed as a reliable model for accurately predicting dendrite growth. However, PF simulations usually require numerical grids that are finer than the dendrite tip curvature radius. Multi-physics simulations of dendrite growth require a computational domain that is larger than characteristic scales such as primary arm spacing, heat and solute diffusion lengths, and solid transport distance. These scales are several orders of magnitude larger than the tip radius, rendering three-dimensional (3D) simulations of dendrite growth particularly challenging. In this study, we combined an adaptive mesh refinement (AMR) method with parallel computing using multiple graphics processing units (GPUs) and developed a *parallel-GPU-AMR* method to perform 3D simulations of dendrite growth. The AMR method dynamically refines the numerical mesh grids around the solid–liquid interface where high spatial resolutions are needed. Our method enabled large-scale simulations with wide primary arm spacings and exhibited good parallel performance [1]. Further, we performed a 3D evaluation of the growth and transport phenomena of the settling dendrite [2]. The developed method is a powerful tool for elucidating the formation mechanisms of solidification microstructures from a multi-physics perspective.

*Keywords: Phase-field method, GPU computing, adaptive mesh refinement method, dendrite growth, solidification.*

[1] S. Sakane, T. Takaki, T. Aoki, Materials Theory 6 (2022) 1–19.
[2] S. Sakane, T. Aoki, T. Takaki, Comp. Mater. Sci. 211 (2022) 111542.

# Augmented Phase-field Model with Finite Interface Dissipation

**Lijun Zhang[1],** Sa Ma[1], Na Ta[1], Shenglan Yang[1], Xiaoke Wu[1], Jia Liu[1], Yuxin Zeng[1]

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**Abstract**

The phase-field model with finite interface dissipation was initially developed by *Steinbach-Zhang-Plapp* in 2012, and later widely used in the materials community, especially in the processes far from the equilibrium state.

In this talk, the major developments in the phase-field model with finite interface dissipation from the past 10 years were first reviewed briefly, including (*i*) the incorporation of the contribution of elastic energy, lastic property, and anisotropy of interfacial energy into the total free energy, as well as the addition of anti-trapping current term; (*ii*) the incorpation of new nucleation model; (*iii*) the effective strategies for coupling with different CALPHAD databases, i.e., thermodynamics, atomic mobility, interface energy, and so on; and (*iv*) the implementation of e.g., GPU parallel computing algorithm. After that, some typical applications of phase-field model with finite interface dissipation in different alloys during various materials processes ranging from solidifcation, solution to aging, were demonstrated. A focus on applications in the additive manufacturing was also presented. Finally, the development directions of the phase-field model with finite interface dissipation the corresponding challenges were pointed. Furthermore, some on-going work on the phase-field model with finite interface dissipation was also given.

*Keywords: Phase-field model with finite interface dissipation; CALPHAD; GPU; Multicomponent alloys; Additive manufacturing*

# Super resolution of three-dimensional microstructural image of a steel using deep learning

**Hoheok Kim**[1], Junya Inoue[2],

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## Abstract

A technique utilizing deep learning is introduced to enhance the resolution of a 3D image of steel microstructures. Typically, a 3D image of a steel sample is obtained through a process involving serial sectioning with a focused ion beam (FIB) and subsequent observation with a scanning electron microscope (SEM). While the FIB-SEM system provides a 3D image of the entire sample, it lacks resolution in the milling direction or the depth direction. To address this issue, a deep learning algorithm based on a super resolution generative adversarial network (SRGAN) is employed to enhance the resolution in the depth direction. This algorithm learns microstructural features from high-resolution surface images and reconstructs low-resolution lateral images, resulting in an upscaled 3D image with improved microstructural details. Experimental results using a low carbon steel sample demonstrate that the deep learning method outperforms conventional techniques, exhibiting the lowest root mean square error (RMSE) among the methods. These findings suggest that the deep learning-based approach is the most realistic and effective means of restoring resolution to images obtained from the FIB-SEM system.

*Keywords: Deep learning, 3d microstructure, steel, super resolution*

# Technical **Oral Session _ Session 7**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 7 (O7)** 10:50 - 11:55, Nov. 22

**Chair :** Xiaobo Chen(RMIT University) 401, 4F

10:50-11:10 **I-O0617** **[Invited] The role of molten salt for sustainable rare metal smelting technology**
Jong-Hyeon Lee (Chungnam National University, Korea)

11:10-11:25 **O-O0666** **Development of an ESR (Electroslag Remelting) simulator to predict chemical reactions during the ESR process for the recycling of high-quality steel scraps**
Jae Hong Shin (Korea Institute of Industrial Technology, Korea)

11:25-11:40 **O-O0734** **Microstructural Analysis and Corrosion Properties of Ni Cladded STS-316H in NaCl+MgCl2 Molten Salt**
Jin Woong Park (Hanbat National University, Korea)

11:40-11:55 **O-O0754** **Recycling titanium scrap via deoxidation of Ti-Ni alloy by Ca and CaCl2-LiF fluxes**
Yao Su (Hanyang University, Korea)

# The role of molten salt for sustainable rare metal smelting technology

**Jonghyeon Lee[1],** Hayk Nersisyan[2], Wanbae Kim[3], Gyuseok Lim[4], Wooseok Choi[5], Donghee Lee[6]

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## Abstract

Rare metal smelting technologies are high-temperature processes using fossil fuels as heat sources or reducing agents. Therefore, a huge amount of greenhouse gas is generated during the metal production process, and alternative process development is actively underway to overcome the problems of the existing smelting process. The electrolytic reduction process has been confirmed as an alternative reduction process for ferrous and non-ferrous metals, but in order to compete with the existing commercial process, it is most important to develop an inert anode material that can secure long-term durability in a high-temperature oxidizing atmosphere.

In this study, we report the development status and experimental results of inert anodes in an environmentally friendly Group 4 metal production process.

*Keywords: Provide a maximum of 5 keywords which appropriately represent the contents of the presentation.*

# Development of an ESR (Electroslag Remelting) simulator to predict chemical reactions during the ESR process for the recycling of high-quality steel scraps

**Jae Hong SHIN**[1], Seounguk BAE[1,2], Minseong KIM[1,2]

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## Abstract

The ESR (Electroslag remelting) process is extensively employed in the refining stage to achieve the production of clean, dense, and homogeneous castings by eliminating undesirable elements and non-metallic inclusions. Nevertheless, when it comes to recycling high-quality steel scraps like mold steel and stainless-steel ingots through the ESR process, there arises a concern regarding the potential loss of valuable alloy elements present in the scrap. This is due to the reaction of oxidative elements in the electrode, such as Al, Ti, and B, with $O_2$ and molten slag during the ESR process, resulting in composition variations between the electrode and the solidified ingot. The conventional methods for predicting and optimizing the chemical composition of the ESR ingot and the slag composition heavily rely on the experience of the operator, incurring significant time, effort, and cost. Hence, the development of an ESR process simulator that takes into account various process variables is crucial to establish customized manufacturing standards and reduce the evaluation time for ESR ingots.
In this study, an ESR process simulator was created utilizing the FactSage macro module, incorporating the concept of Effective Equilibrium Reaction Zone.The developed simulator successfully predicted changes in the chemical composition along the length direction of the ingot and identified the types of inclusions.

*Keywords: ESR process, Simulation, Recycle of scrap, Slag, Effective Equilibrium Reaction Zone*

# Microstructural Analysis and Corrosion Properties of Ni Cladded STS-316H in NaCl+$MgCl_2$ Molten Salt

**Jin Woong Park[1],** UiJun Ko[1], Ji-Hyun Yoon[2], Jeoung Han Kim[1*]

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## Abstract

Molten salt reactors (MSRs) have gained attention due to their potential safety, sustainable fuel cycles, and high salt melting and boiling points. Operating at high temperatures and atmospheric pressure, MSRs offer potential cost advantages. This study explores the application of nickel (Ni) cladding on stainless steel (STS) surfaces in MSRs to enhance corrosion resistance and mechanical properties. Nickel's excellent corrosion resistance in molten salt environments makes it suitable for cladding applications which serves as a protective barrier, reducing corrosion rates and extending the material's service life. Present study focuses on the investigating the corrosion performance and microstructure of laser-cladding of Ni on STS-316H in NaCl+$MgCl_2$ molten salt. Pure Ni was cladded on STS-316H via both wire-overlay and laser deposition methods. Results indicate that the molten salt corrosion performance depends on both the thickness of the Ni layer and microstructural characteristics, such as grain size, Cr atoms diffusion distance, defects, and the presence of second-phase particles. Furthermore, the Ni cladding enhances mechanical properties, including strength and hardness, crucial for structural integrity under high-temperature and high-stress conditions. The findings contribute to understanding the potential benefits of Ni-cladded STS in MSR applications, aiding further research and development in this field.

*Keywords: Molten salt, Corrosion, Ni-cladding, STS316, Molten salt reactor(MSR)*

# Recycling titanium scrap *via* deoxidation of Ti-Ni alloy by Ca and $CaCl_2$-LiF fluxes

**Yao Su[1],** Sheng-chao, Duan[1], Min-Joo, Lee[1], Yeong-Jin, Jun[1], Kwang-Seok Park[2], Joo Hyun PARK[1,*]

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## Abstract

The present study investigates the possibility of the direct removal of oxygen from the Ti-Ni alloy melt through the thermodynamic equilibrium reactions at 1723 K in the vertical tube furnace. The deoxidation efficiency of Ti-Ni alloy melt by adding different content of metallic calcium (Ca) as a deoxidant was evaluated with the binary halide flux of calcium chloride and lithium fluoride. The thermodynamic equilibrium experiments showed that when 0.9 wt% Ca was added to the Ti-Ni alloy, the total oxygen content in the alloy decreased from about 530 ppm (initial value) to 400 ppm. The equilibrium constant of the deoxidation reaction and the interaction parameter between calcium and oxygen were determined for the Ti-Ni alloy at 1723 K.

Alternatively, the effect of different flux compositions, i.e., LiF/$CaCl_2$ ratio in the $CaCl_2$-LiF binary flux on the oxygen content was also investigated at 1723 K. According to the results, the flux system with 25%LiF – 75%$CaCl_2$ showed a good deoxidation capability, the total oxygen content in the alloy reduced from 900 to 670 ppm.

*Keywords: Titanium scrap, Ti-Ni alloy, Deoxidation, Calcium, Halide flux*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 8

November 22

14:00-15:30

# Technical **Oral Session _ Session 8**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 8 (A8)** **14:00 - 15:45, Nov. 22**

**Chair :** To be announced Halla Hall A, 3F

14:00-14:30 **K-A0373** **[Keynote] Mechanical Property Analysis of High Strength Steels by Neutron Diffraction Experiments**
Noriyuki Tsuchida (University of Hyogo, Japan)

14:30-14:50 **I-A0605** **[Invited] Understanding of liquid metal embrittlement cracks (LME) in Zn-coated resistance spot welding : Electrode contact and nugget growth for stress development and cracking**
Yeong-Do Park (Dong-Eui University, Korea)

14:50-15:10 **I-A0232** **[Invited] Microstructural characterization using advanced small-angle scattering**
Yojiro Oba (Toyohashi University of Technology, Japan)

15:10-15:30 **I-A0794** **[Invited] Toughening ultrastrong steel by textured δ-ferrite lamellas**
Haiwen Luo (University of Science and Technology Beijing, China)

15:30-15:45 **O-A1167** **Prior austenite refinement route and precipitation regulation for 1 GPa grade high-strength high toughness low alloy steel**
Zhenjia Xie (University of Science and Technology Beijing, China)

# Mechanical Property Analysis of High Strength Steels by Neutron Diffraction Experiments

**Noriyuki Tsuchida**[1]

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## Abstract

Steels are often used as multi-phase or multi-microstructure steels, composed of multi phases and microstructures. Information on the deformation behavior of phase and grain units is very beneficial for understanding the mechanical properties of steel. Neutron diffraction experiments can provide such the information on the deformation behavior of phase and grain units during tensile deformation in terms of phase strain and lattice strain. The presenting author has conducted *in situ* neutron diffraction experiments during the tensile deformation of various steels with different strength levels to investigate the important factors that improve mechanical properties. In this study, the author will focus on the results of neutron diffraction experiments on high-strength steel plates obtained so far.

*Keywords: High-strength steels, lattice strain, phase strain*

# Understanding of liquid metal embrittlement cracks (LME) in Zn-coated resistance spot welding : Electrode contact and nugget growth for stress development and cracking

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## Abstract

Liquid metal embrittlement (LME) cracking is one of the difficulties when Zn-coated advanced high strength steels (AHSS) are joined with resistance spot welding (RSW). The danger of this cracking could be magnified in case of 3rd generation AHSS owing to the high alloying content (Mn and Si) in the proposed alloys designs (Q&P, Med. Mn and TBF). This talk aims at the understanding of the mechanism of Zn-assisted LME cracking and hence proposing various approaches to control it. The experimental and simulation results revealed that the LME cracks are concentrated at certain weld locations owing to the synergetic effect of temperature, stress, time of exposure to liquid zinc, and time of exposure to tensile stress at the corresponding locations. A mechanistic model with nugget growth rate and electrode contact growth was proposed and verified through cross-comparison of LME observations. In conclusion, this research provides valuable insights into the critical stages of LME cracking during RSW of Zn-coated steel and suggests ways to mitigate this issue.

*Keywords: Liquid metal embrittlement crack, Resistance spot welding, 3rd generation advanced high strength steel, Thermal gradient.*

# Microstructural characterization using advanced small-angle scattering

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**Abstract**

Precise characterization and control of microstructures become more and more important for the development of advanced steels to further improve mechanical and physical properties. Small-angle scattering is a powerful means for the microstructural characterization ranging mainly from a few μm to 1 nm. Inclusions and precipitates are included in this size range and have been frequently targeted by both small-angle X-ray scattering (SAXS) and neutron scattering (SANS). The quantitative information provided by SAXS and SANS is beneficial to the comparison of the change in the microstructures and often plays a key role to clarify precipitation mechanisms. In addition, recent progress of SAXS and SANS techniques allows to obtain more information. Anomalous SAXS (ASAXS) can measure the microstructures of a specific element in samples and is an established experimental method. In addition, state-of-the-art synchrotron beamlines make it easy to access ASAXS. In SANS, magnetic scattering contribution can be used to enhance the weak scattering signal from fine precipitates. The analysis techniques combined with micromagnetics enables the detailed analysis of magnetic microstructures. This is also useful to investigate crystal defects, which have different magnetic properties from matrix.

*Keywords: small-angle X-ray scattering, small-angle neutron scattering*

# Toughening ultrastrong steel by textured δ-ferrite lamellas

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## Abstract

By both the standard Charpy V-notched impact and projectile tests, we here investigated the dynamic fracture behaviour of a recently developed ultrastrong lightweight steel comprising a hierarchical martensitic matrix, dispersed ultra-fine-retained austenite grains and oriented δ-ferrite lamellas, the latter being due to high Al and Si contents employed for low-density design. This steel shows a superior combination of specific ultimate tensile strength and impact toughness to other ultrastrong steels and has successfully arrested a real steel-cored bullet shot. These are attributed to the densely textured δ-ferrite lamellas that can deflect the propagating cracks until they are trapped and enclosed besides austenite-to-martensite transformation crack closure, leading to more energy consumed before failure. These results suggest a new pathway for toughening ultrastrong lightweight steels.

*Keywords: ultrahigh strength, low density steel; δ-ferrite lamellas; crack propagation; toughness.*

# Prior austenite refinement route and precipitation regulation for 1 GPa grade high-strength high toughness low alloy steel

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**Abstract**

Quenching and tempering processing has been wildly used to produce high strength high toughness steels. Obtaining fine and homogeneous prior austenite grains during reaustenitization before quenching is very important for both high strength and high toughness. In-situ high-temperature EBSD characterization was carried out to directly observe reaustenitization in a low alloy steel with different initial microstructures. For lath martensite/lower bainite, globular austenite mainly nucleated at prior austenite grain boundaries, and grew gradually to form uniform small grains from 780 to 860˚C. For granular bainite, martensite-austenite constituents accelerated acicular austenite formation via martensitic reversion transformation. Then, acicular grains coalesced, resulting large grains. Furthermore, the effect of tempering temperature on carbides and toughness was systematically studied. It is found that less carbides precipitated at low temperature of 200-450˚C, leading to similar toughness to the quenched steel. After tempering at 500-600˚C, a huge number of acicular carbides precipitated, resulting dramatically decrease in toughness of the studied steel at no obvious cost of strength. When further increasing tempering temperature to 620-660˚C, the precipitated carbides were almost in spherical or rod-like in size of less than 150 nm, the toughness were significant enhanced with slightly decrease in strength. Benefited from grain refinement and carbides regulation, yield strength of 960 MPa with excellent low temperature toughness was obtained in this work.

*Keywords: 1GPa low alloy steel, grain refinement, carbide regulation, thigh toughness*

# Technical **Oral Session _ Session 8**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 8 (B8)** **14:00 - 15:20, Nov. 22**

**Chair :** Robert Wilson (CSIRO Manufacturing), Hwijun Kim (Korea Institute of Industrial Technology) **301, 3F**

14:00-14:20 **I-B0740** **[Invited] Stress corrosion cracking behavior of the high strength steels**
Hyokyung Sung (Kookmin University, Korea)

14:20-14:35 **O-B0021** **Synopsis of an auto-leveling-control system of tandem HSM base on predictive theoretic model with stainless steel strip rolling practice**
Li Huifeng (Baowu Iron & Steel Group Taiyuan Iron & Steel Company, China)

14:35-14:50 **O-B0039** **Research on Collaborative Control Technology of Color Difference and Flat Coil Defects of Advanced High Strength Steel**
Lin Wang (Research Institute of Technology, Shougang Group Co., Ltd., China)

14:50-15:05 **O-B0095** **Control of MnS Morphology during Billet Casting and Hot Rolling of Ultra-High Sulfur Medium Carbon Steel**
Lyu Naibing (Research Institute of Technology, Shougang Group Co., Ltd., China)

15:05-15:20 **O-B0146** **Effect of initial grain size on microstructure, texture, and magnetic properties of non-oriented electrical steel**
Zhen Wang (University of Science and Technology Beijing, China)

# Stress corrosion cracking behavior of the high strength steels

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## Abstract

This study aims to reveal the atomic-scale effects of tempering, carbon redistribution, and associated precipitates on the complex substructures, stress corrosion cracking (SCC) resistance, and tensile properties of high-sustainability martensitic steels. The SCC resistance, corrosion potential, and strength of boron-doped martensitic steel increase concurrently without the need for low-temperature tempering. Notably, the degradation of SCC resistance and corrosion potential induced by tempering contrasts with the known effect of tempering. To explore this unprecedented result, subboundaries within the martensitic microstructure are investigated through atomic-nano-micro-scale bridging analyses via transmission Kikuchi diffraction, transmission electron microscopy, and atom probe tomography. Similar to the typical tempering effect, tempering promotes both lath coarsening and more blocks within a single martensitic grain, resulting in a decreased dislocation density and residual stress, and consequently, decreased strength and increased elongation. Contrary to the trend where blocks are a key strengthening mechanism, the lath boundary is crucial for SCC resistance and corrosion potential. Although boron atoms with similar compositions are mostly segregated at the prior austenite grain boundaries regardless of tempering, more carbon is present at the lath boundaries in tempered martensite. The strongly segregated carbon during tempering acts as a precursor to the increased density and size of harmful cementite, which act as severe SCC initiation sites. Eventually, tempering causes intensive crack growth along the lath boundaries, deteriorating the material's sustainability.

*Keywords: Stress corrosion cracking, high-strength steels, martensite, grain boundary segregation*

# Synopsis of an auto-leveling-control system of tandem HSM base on predictive theoretic model with stainless steel strip rolling practice

**Huifeng Li**[1] Zhongjie Wang[2] Jianmin Li[3] Zhong Wang[4]
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**Abstract**

An auto-leveling-control system of tandem HSM was developed by researchers from Shanxi University and Baowu Iron & Steel Group Taiyuan Iron & Steel Company, to acquire improved straightness of hot-rolled strip with better coil shape. To each pass of the rough mill, and each finishing mill, a group of leveling value was calculated with an initiative theoretic model previously based on parameters and technology data collected from the sites, which is sent to hydraulic leveling system, triggered by corresponding event signal while the rolling process taken place, to eliminate wedge difference along the piece to get a controllable straightness. The auto-leveling-control system were applied in the 2250 tandem HSM while producing strip of 400 series stainless steel, with significant performance in rolling stability, strip straightness, coil shape, and surface defects control.

*Key words: HSM, auto leveling control, system, strip, coil shape*

# Research on Collaborative Control Technology of Color Difference and Flat Coil Defects of Advanced High Strength Steel

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## Abstract

Color difference and flat coil defects are common industry problems at home and abroad for advanced high strength steel, and its popularization is therefore limited.Existing mechanism research and control measures of the two defects have encountered problems in practice,and it's difficult to control both types of defects at the same time. This study extends the classical theory of red scale defects of Japanese Scholars,micro-cracks in the surface layer of cold-rolled strip is found as the direct cause of the color difference defect. Comprehensive control means including slab heating,descaling,hot rolling and cold rolling process are proposed. Color difference defects and related red scale defects are effectively controlled.However, some measures are inconsistent with the conventional control of flat coil defects.Therefore, the relationship between hot rolling process, phase transformation and flat coil defect is studied in detail.Based on theoretical research, a combined hot coil cooling method including ultra fast cooling is proposed and successfully applied in production practice,the expansion amount of phase transformation before hot coiling is greatly reduced and the micro-cracks in the surface are suppressed,thus the flat coil defect and color difference defect are effectively controlled simultaneously.The surface quality and coil shape quality of Shougang advanced high strength steel have been greatly improved.

*Keywords: Color difference;Flat coil defect;Advanced high strength steel;Micro-cracks;Phase transformation*

# Control of MnS Morphology during Billet Casting and Hot Rolling of Ultra-High Sulfur Medium Carbon Steel

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## Abstract

In order to obtain spindle MnS inclusions in hot-rolled ultra-high sulfur medium-carbon steel wire rod, the generation, growth and elongation of MnS in the product was analyzed by using the second phase precipitation theory, billet solidification numerical simulation calculation and thermal simulation experiments. The three-dimensional morphology of MnS inclusions was obtained by Synchrotron Radiation Facility. Results show that MnS was generated at the end of the solidification in cast billet when solid phase fraction fs=0.446 with the segregation ratio of S reaches 2.19. The growth process of MnS during solidification determines the diameter of the MnS particles in the billet. Hot rolling temperature and deformation amount affects the elongation of MnS.The theoretical calculation shows that when the secondary cooling water volume is fixed to 0.6L/kg the MnS in the 160mm² billet center grows up to 30.6, 32.2and 34.6μm at the casting speed of 1.6m/min, 2.1m/min and 2.6m/min respectively, which is consistent with the actual test results. The key to controlling the size of MnS in wire rod is to increase the cooling intensity of the secondary cooling zone and reduce the casting speed of the billet. Based on the calculation method in this paper control range of continuous casting process parameters matching the MnS diameter in 160mm² billet is presented.The most favorable rolling deformation should be 30% with the rolling rate between 0.45$s^{-1}$ and 0.78$s^{-1}$ under the temperature between 1050℃ and 1100℃ to limit the MnS elongation.

*Keywords: MnS growth;super high S content;medium carbon free-cutting steel.*

# Effect of initial grain size on microstructure, texture, and magnetic properties of non-oriented electrical steel

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## Abstract

Non-oriented electrical steels (NGO) are widely used as core materials in motors, generators, and sensors due to their excellent soft magnetic properties. The magnetic properties of NGO are influenced by silicon content, grain size, texture, and impurities. Numerous studies have shown that the texture is inherited, and the initial grain size, particularly, prior to cold rolling has a notable effect on the magnetic properties. Therefore, it is crucial to study the mechanism of the influence of the initial microstructure on the structure and texture of NGO for the optimization of its magnetic properties.

Fe-3.5 wt% Si NGO was prepared via varying parameters and process routes, in order to investigate the effect of initial microstructure before cold rolling on the magnetic properties. It was found that the initial grain size had a significant influence on microstructure, texture evolution, and magnetic properties. There were large and massive shear bands in the sheet with coarse initial grains, after cold rolling, which led to λ and {113}<631> oriented grains concentratedly nucleated during the early stage of recrystallization. The {113}<631> grains had significant growth advantage, resulting in sharp α*-fiber texture in the final annealed sheet. Stronger α*-fiber texture and weaker γ-fiber texture both promoted the optimization of magnetic properties. As a result, the magnetic induction $B_{50}$ was 1.719T, and core loss $P_{15/50}$ was 2.69 W/kg, $P_{10/400}$ was 16.337 W/kg.

*Keywords: non-oriented electrical steel, grain size, texture, magnetic property*

# Technical **Oral Session _ Session 8**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 8 (C8)** **14:00 - 15:35, Nov. 22**

**Chair :** Elena Pereloma (University of Wollongong ), Hiroyuki Yasuda (Osaka University) 201A, 2F

14:00-14:30 **K-C0762** **[Keynote] Oxidative Influence on Tensile Properties of TiAl Intermetallic and Ni-based Alloys: Comparative Review**
Ji ZHANG (Central Iron & Steel Research Institute, China)

14:30-14:50 **I-C0757** **[Invited] Investigation of the effect of cooling rate after heat treatment on creep properties of single crystal superalloy**
Jeonghyeon Do (Korea Institute of Materials Science, Korea)

14:50-15:05 **O-C0433** **γ′-Strengthened Multicomponent CoNi-Based Wrought Superalloys With Improved Comprehensive Properties**
Song Lu (University of Science And Technology Beijing, China)

15:05-15:20 **O-C0490** **Development of Temperature Estimation Method for KA-SUS321J1HTB using σ -phase Particle Size**
Masahito Omiya (IHI Corporation, Japan)

15:20-15:35 **O-C0932** **Enhancement of strength-ductility trade-off in directionally solidified Al-rich Ni-27Al alloy via particle reinforced composite structure formation by static magnetic field**
Sansan Shuai (Shanghai University, China)

# Oxidative Influence on Tensile Properties of TiAl Intermetallic and Ni-based Alloys: Comparative Review

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## Abstract

Structural materials for engine applications are repeatedly exposed to air at elevated temperatures so that oxidation layers always form in the surfaces which are potentially harmful to the mechanical properties as the crack nucleation sites. At mean time, oxidation-related microstructure degradation such as formation of strengthening elements or precipitates depleted region can also affect the components' bearing capacity. This talk try to assess the tensile characteristics of a TiAl intermetallic alloy and a solid solution strenthening Ni-based GH 3230 alloy ever subjected to oxidative influences. Some highlights includes that the the oxidation always produces an embrittlement surface layer in TiAl alloys and causes the signicant loss of the ductility only when the alloys contain the lamellar structures with monolithic orientation. By contrast, the ductile layer generates in the surface of GH 3230 alloy due to the oxidation depletion of strenthening elements and carbides dissolution during cyclic thermal exposure process that leads to the good tensile property retention. It is also worth noting that the minor alloying additions of La and Mn are found beneficial to the oxide adhesion and therefore helpful to further diminish the strength loss from the outer scale spallation.

*Keywords: TiAl intermetallic alloy, GH 3230 alloy, oxidation, tensile property.*

# Investigation of the effect of cooling rate after heat treatment on creep properties of single crystal superalloy

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## Abstract

Ni-based single crystal superalloys are alloys having excellent properties at high temperatures and are manufactured using a single crystal casting process such as the Bridgman casting method. In general, Ni-based single crystal superalloys are sequentially subjected to solution heat treatment and aging heat treatment in order to grow strengthening phase γ′ uniformly after single crystal casting. Therefore, it is known that the cooling rate of solution heat treatment does not significantly affect on the microstructure and creep property. However, it was confirmed that the creep property of a specific single crystal superalloy vary greatly depending on the cooling rate after solution heat treatment. In this study, it was inferred that the difference in creep properties due to lattice misfit, and the effect of cooling rate after solution heat treatment on lattice misfit was investigated. In order to accurately calculate the lattice misfit, the lattice constants were measured using the high-resolution XRD and the APT analysis method. It was confirmed that the absolute value of the lattice mismatch increased as the cooling rate increased, and this result was consistent with the result that the creep characteristics improved dramatically as the cooling rate increased.

*Keywords: Single crystal superalloy, Creep, lattice misfit*

# γ′-Strengthened Multicomponent CoNi-Based Wrought Superalloys With Improved Comprehensive Properties

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## Abstract

The discovery of γ′-strengthened Co-based alloys has opened a new avenue for developing high-temperature structural materials applied in industrial turbine blades and disks. Previous research has demonstrated that γ′-strengthened CoNi-based wrought superalloys have a potential advantage in hot workability due to the relatively lower γ′ solvus temperatures compared to those of advanced Ni-based wrought superalloys. To accelerate the adoption of γ′-strengthened CoNi-based wrought superalloys in engineering applications, we designed and optimized alloys for microstructural stability, hot workability, oxidation resistance, and density, using an accelerated framework that integrated multicomponent diffusion-multiples and machine learning. The multicomponent diffusion-multiples allowed for a collection of a large amount of experimental data related to composition and microstructural parameters. Machine learning enabled the exploration of the effects of alloying elements on microstructural stability and parameters. Multicomponent CoNi-based superalloys with high Cr content were designed to possess a γ/γ′ two-phase microstructure with a relatively high γ′ volume fraction (≥ 45%), low γ′ coarsening rate, and spherical or cuboidal γ′ morphology. The optimal alloys' phase transformation temperatures, microstructural stability, oxidation resistance and mechanical properties were evaluated and compared to other CoNi-based and Ni-based wrought superalloys. This framework and the insights obtained will assist in accelerating the development and engineering application of multicomponent CoNi-based superalloys.

*Keywords: CoNi-based superalloys, Alloying effects, Microstructural design, Multicomponent diffusion-multiple, Machine learning*

# Development of Temperature Estimation Method for KA-SUS321J1HTB using σ -phase Particle Size

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## Abstract

Austenitic stainless steels are used for boiler heat transfer tubes in the thermal power plants. Since these tubes are exposed to high temperature and internal pressure for over 100,000 hours and crept, there is a strong demand for the remaining life assessment method. The operating condition of the boiler tubes, such as temperature, internal pressure and service time are necessary for the creep life assessment. Previously, the authors developed a temperature estimation method of austenitic stainless steels using the relationship between σ phase particle size and Larson-Miller parameter (LMP). We have confirmed that this method is applicable for KA-SUS304J1HTB.

KA-SUS321J1HTB is also an austenitic stainless steel used for the boiler tubes, but we didn't confirm whether this method is applicable for KA-SUS321J1HTB. In this study, therefore, the applicability of the above method for KA-SUS321J1HTB was investigated. Creep rupture tests were conducted under various temperature and stress levels. The average σ phase diameter was measured at the gauge and head portion of ruptured specimens. It was found that σ phase precipitated earlier at the gauge portion compared to the head portion. It was suggested that the stress promoted σ phase precipitation in KA-SUS321J1HTB. In contrast, there was no significant difference in the average σ phase diameter between the gauge and head portion. The averages of σ phase diameter at the gauge and head portion were explained with a single curve as a function of LMP. It is expected that operating temperature of KA-SUS321J1HTB boiler tubes can be predicted using this curve.

*Keywords: Austenitic stainless steel; σ phase; Creep; Temperature estimation*

# Enhancement of strength-ductility trade-off in directionally solidified Al-rich Ni-27Al alloy via particle reinforced composite structure formation by static magnetic field

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## Abstract

As one of the ideal materials for the next generation of turbine blades, Al-rich β ( NiAl ) / γ' ($Ni_3Al$) two-phase $Ni_3Al$ alloy has the advantages of low density and high service temperature, but its low plasticity at room temperature makes it inapplicable. In this paper, the directional solidification process of Ni-27Al alloy is controlled by applying a static magnetic field, and a new composite structure with refined equiaxed β phase uniformly dispersed in the single crystal γ′ matrix is obtained, which simultaneously improves its room temperature strength and plasticity. The β-phase particles maintain a certain preferred orientation after breaking under low magnetic field, while the orientation of the γ′-phase matrix is not affected, thus forming a new composite structure material composed of oriented β-phase particles and single crystal $Ni_3Al$ phase matrix. Accordingly, the yield strength, tensile strength and elongation of Ni-27Al alloy at room temperature reach 307.5MPa, 525.6MPa and 8.2%, which are 13.7%, 16.6% and 49% higher than those without magnetic field, respectively. Based on this specific composite structure, the interfacial properties and slip transfer mechanism between the two phases realise the excellent combination of strength and plasticity of the alloy. This paper provide a new method to regulate the microstructure of β / γ' two-phase $Ni_3Al$-based alloys under static magnetic field and improve the mechanical properties of strength and toughness, which enable to break the application bottleneck of high-performance $Ni_3Al$ alloys.

***Keywords:*** *Ni-27Al alloy; Magnetic field; Directional solidification; Mechanical properties, composite structure.*

# Technical **Oral Session _ Session 8**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 8 (D8)** **14:00 - 15:35, Nov. 21**

**Chair :** Kazumasa Yamazaki (Nippon Kinzoku Co., Ltd) Samda Hall A, 3F

14:00-14:20 **I-D0790** **[Invited] Overview of Advancement and Development Trend on Magnesium Alloys based on《Journal of Magnesium and Alloys》**
Xiaodong Peng (Chongqing University, China)

14:20-14:35 **O-D0765** **STEM Characterization of Solute Segregation and Segregation-induced/associated Precipitation in Light Alloys**
Jian-Feng Nie (Monash University, Australia)

14:35-14:50 **O-D0875** **Study of kink formation mechanism in compressed Mg alloys with LPSO phase with CPFEM simulations**
Yu Shen (University of Tokyo, Japan)

14:50-15:05 **O-D0345** **Persistent homology and 3D strain analyses of Mg/LPSO two-phase alloys**
Daiki Kuriki (The University of Tokyo, Japan)

15:05-15:20 **O-D0580** **Establishing role of microstructural engineering on strain gradient plasticity of a rare earth containing magnesium alloy**
Sourav Mishra (Indian Institute of Technology Madras, India)

15:20-15:35 **O-D0619** **The multi-solute solid solution behavior of magnesium alloys and their application on materials design**
Yuan Yuan (Chongqing University, China)

# Overview of Advancement and Development Trend on Magnesium Alloys based on 《Journal of Magnesium and Alloys》

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## Abstract

Magnesium alloys have become an important lightweight metallic structural material and have been widely studied worldwide. As the only journal focusing on magnesium alloy research which devoted to the coverage and dissemination of global research on magnesium alloys, Journal of Magnesium and Alloys provides an international medium for the publication of theoretical and experimental studies in magnesium science and engineering. Journal of Magnesium and Alloys covers all aspects of magnesium and alloys and their manufacture, including raw materials, alloy casting, extrusion and deformation, corrosion and surface treatment, joining and machining, simulation and modeling, microstructure evolution and mechanical properties, new alloy development, magnesium-based composites, bio-materials and energy materials, applications, and recycling. This topic statistically analyzes all the academic articles published by Journal of Magnesium and Alloys from 2013 to 2022 and compares them with all the articles containing magnesium alloy in their titles on the Web of Science during this period. The development trends of magnesium alloys are summarized based on these articles, and the influence and academic value of the articles published by the Journal of Magnesium and Alloys are summarized as well. This topic hopes to better realize the value of JMA, help better spread the academic research of magnesium alloys, and promote the development of global magnesium alloy research.

***Keywords:*** *Magnesium alloy; developing trend; research hotspots;*

# STEM Characterization of Solute Segregation and Segregation-induced/associated Precipitation in Light Alloys

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## Abstract

The limit for your abstract is 250 words. Do not include tables, formulae, and equations.

Mechanical properties of light alloys are strongly influenced by the distribution of solutes, clusters of solutes, and precipitates. While conventional transmission electron microscopy has been used for several decades, the atomic scale information regarding the distribution of atoms of micro-alloying elements in solute clusters, precipitates and precipitate-matrix interfaces remains unclear in many cases. Furthermore, the formation mechanisms of precipitate plates are still a subject of controversy, leading to speculation about the roles of micro-alloying elements in precipitation of key strengthening precipitate phases. However, recent advancements in aberration-corrected scanning transmission electron microscopy (STEM) have provided opportunities to detect segregated solute atoms and solute clusters at the atomic scale. By combining these techniques with atomic-scale computations, it becomes possible to reveal the mechanisms behind precipitate formation. The objective of this presentation is to provide an overview of recent studies conducted by using atomic-resolution STEM imaging and mapping techniques, as well as first-principles computations, to investigate solute segregation and segregation-induced/associated precipitation in selected aluminium, magnesium and titanium alloys.

*Keywords: HAADF-STEM, solute segregation and precipitation, Mg, Al, Ti*

# Study of kink formation mechanism in compressed Mg alloys with LPSO phase with CPFEM simulations

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## Abstract

The Mg alloy incorporating a long period stacking order (LPSO) phase is presently under investigation as a potential lightweight structural material of promise. Given that the superior strength of the Mg/LPSO alloy is primarily attributed to kink formation in LPSO phase [1], becomes imperative to delve into the kink formation mechanism in LPSO phase to further enhanc the strength of the LPSO alloy. While it might be expected that the LPSO phase, which boosts th strength of the Mg alloy, has greater strength and would deform after the deformation of the M phase to maintain the high strength of the whole alloy, Digital Image Correlation (DIC) analysi in this study shows a different pattern. Strain mainly concentrates within and close to the LPS phase at the start of compression, suggesting that deformation first happens in the LPSO phase i the dual-phase alloy. To understand this phenomenon and gain deeper insights into the deformatio mechanism of kink deformation, the Crystal Plasticity Finite Element Method (CPFEM) is use to simulate strain partitioning during the compression test.

The impact of the critical resolved shear stress (CRSS) of the basal slip and prismatic slip in bot the Mg phase and LPSO phase is studied in CPFE simulations. DIC, which shows the strai partitioning of the alloy, is used to validate the CPFE model. At the same time, Scanning Electro Microscopy (SEM) is conducted to observe changes in microstructure and kink morphology, providing further support for the model.

*Keywords: Magnesium alloy, Kink deformation, Microstructure, DIC, CPFEM*

[1] K. Hagihara et al, Acta Materialia, 163(2019) 226-239.

# Persistent homology and 3D strain analyses of Mg/LPSO two-phase alloys

**Daiki Kuriki**[1], Fabien Briffod[1], Takayuki Shiraiwa[1], Manabu Enoki[1]

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## Abstract

Mg/LPSO two-phase alloys, which consist of soft Mg phases and hard long-period stacking ordered (LPSO) phases, are expected to be the next-generation structural materials due to their excellent properties. In recent years, efforts to observe the fracture process of metallic materials in three dimensions (3D) have become active due to the development of X-ray CT equipment. In particular, the usefulness of 3D observation has been demonstrated in materials with complex structures such as those with multiple phases, where detailed fracture mechanisms that could not be elucidated in two dimensions can be revealed.

This study aimed to elucidate the relationship between microstructure and deformation behavior of Mg/LPSO two-phase alloys using X-ray CT. In addition to qualitative observations, digital volume correlation (DVC) was applied to 3D microstructure images before and after the compression test to measure the 3D strain distribution generated by deformation. Furthermore, using data-driven approaches to analyze large amounts of data on microstructure images obtained by X-ray CT and strain distribution obtained by DVC, the characteristics of microstructures that are prone to high strain were investigated. Specifically, a machine learning model was developed to predict strain values from microstructural descriptors extracted from microstructure images, and inverse analysis of the model was also performed. The study found that regions with high connectivity in the LPSO phase were more prone to high strain, as evidenced by the use of persistent homology, a descriptor that can describe the connectivity of the microstructure.

*Keywords: Mg/LPSO two-phase alloys, Three-dimension, Digital volume correlation, Data-driven, Persistent homology*

# Establishing role of microstructural engineering on strain gradient plasticity of a rare earth containing magnesium alloy

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Magnesium (Mg) and its alloys have potential applications in sheet metal parts of several automotive, aerospace, electronics and biomedical industries owing to their excellent light weighting properties. To meet these applications, bendability of magnesium alloy sheets constitutes a fundamental requirement to be achieved for improving its manufacturability. However, presence of strain gradients during bending operation, inherent tension compression yield asymmetry in Mg alloys and their micromechanical deformation mechanisms play a crucial role in determining efficiency of bending operation. The current study is focused towards understanding the influence of refining the grain size on yield asymmetry and its influence on extension twinning (as a micromechanical deformation mechanism) during bending of Magnesium alloys. A combination of severe plastic deformation (SPD) and post-SPD annealing treatments were used to engineer several grain sizes in a Rare Earth containing Mg alloy. Sheet metals with varying microstructural grain sizes were subjected to a predefined displacement limit during the bending operation. Role of deformation mechanisms such as extension twinning was established through electron microscopy-based characterization of bent Mg alloy sheet metal samples. The detailed scientific know-how of micromechanical deformation behavior was established and correlated to yield asymmetry ratios and overall sheet metal bendability of the engineered Mg alloys.

*Keywords: Magnesium alloys, Bendability, Strain Gradients, Micromechanical deformation, Severe Plastic Deformation, Microstructure*

# The multi-solute solid solution behaviour of magnesium alloys and their application on materials design

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**Abstract**

The low-density magnesium (Mg) alloys are attractive for the application in aerospace, transportation and other weight-saving-required fields. It is noteworthy that the solid solution of alloying elements in the α-Mg phase can have multi-effects on the properties of Mg alloys, e.g, solid solution strengthening, solid solution corrosion-resistance-enhancing, etc. And it is also notably the functional properties, e.g. damping capacities, magnetic shielding properties can also be tailored by controlling the solution in the matrix. It is promising that by selected proper multi-alloying-elements (with optimal ratio) solid solution in the α-Mg phase, the comprehensive properties of Mg alloys can be synergy improved. In this work, the solid solution behaviour of Mg alloys and the followed solid solution property-enhancing effects were studied. Three types solution behaviour in the ternary magnesium alloy systems were proposed and the application for the materials design for specified functions were proposed.

**Presenting author**: Professor of Chongqing University, Marie-Curie Fellow, being in Editor Board of International Journal Materials Science, Junior Editor of Journal Magnesium and Alloys, majoring in materials calculation and design, Principle Investigator of national key projects and EU projects, have around 70 publications and 20 invited talks.

*Keywords: Magnesium alloys; Thermodynamics; Materials design.*

# Technical **Oral Session _ Session 8**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 8-1 (E8-1)** **14:00-15:30, Nov. 22**

**Chair :** Mahyar Khorasani (Royal Melbourne Institute of Technology) Halla Hall B, 3F

14:00-14:30 **K-E0503** **[Keynote] Computational developments in design for additive manufacture, lowering the certification bar: a Defence perspective**
Christopher Wallbrink (The Defence Science and Technology Group (DSTG), Australia)

14:30-14:45 **O-E0507** **Effect of compression direction on the hot deformation and microstructure evolution of selective laser melted 718 alloy**
Wei Le (Northwestern Polytechnical University, China)

14:45-15:00 **O-E0669** **A Simple Detection Method of Microdefects during Metal Additive Manufacturing Process Using Acoustic Emission Monitoring**
Kaita Ito (National Institute for Materials Science, Japan)

15:00-15:15 **O-E0713** **Development of Low-Cost Ti-6Al-4V Filler Wire Manufacturing Process for Wire Arc Additive Manufacturing**
Anoop Maurya (Korea Institute of Materials Science, Korea)

15:15-15:30 **O-E0867** **A multi-scale numerical and experimental study for solidification microstructure and defects of superalloys fabricated by selective laser melting additive manufacturing**
Songzhe Xu (Shanghai University, China)

# Computational developments in design for additive manufacture lowering the certification bar: a Defence perspective

**Chris Wallbrink**

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## Abstract

The Defence enterprise has a strategic need to be across new technologies that could lead to a capability edge. Advance manufacturing is a key enabler facilitating the development of new materials and technologies that support the future Defence force. What is evident in the development of this new capability is the growing complexity of novel advanced manufacturing technologies and associated challenges. Challenges include new material behaviours, manufacturing specific defects and limitations in design freedom. Hence, novel technologies require novel approaches to realise their benefits. Considerations of material selection, multi-objective optimisation and manufacturing constraints are important in design, but are areas where computational gaps persist. The Defence Science and Technology Group (DSTG) is working with Defence partners, academia and industry to actively develop computational tools to expedite material discovery and enable rapid design prototyping to leverage new manufacturing technologies. Examples in powder bed and laser metal deposition additive manufacturing (AM) are used to showcase computational capabilities currently in development at DSTG. These computational capabilities augment the existing traditional commercial off the shelf products and traditional design philosophies used in the development life cycle. Specific examples will be presented for a structural aerospace component with further discussion around the influences of material properties. Although the capabilities are domain agnostic, the presentation focuses on structural design for aerospace application. Structural certification of AM components remains a significant industry challenge and DSTG's computational efforts to aid certification of replacement components are presented. Further, emerging capabilities in material characterization at the micron level and approaches to integrate this capability at the component level design are discussed. While challenges remain, DSTG's efforts in computational design demonstrate clear advances in lowering the bar to structural certification.

*Keywords: Computational Tools, Additive Manufacture, Certification, Structural Design*

# Effect of compression direction on the hot deformation and microstructure evolution of selective laser melted 718 alloy

**Wei Le[1],** Zhongwei Chen[2], Kang Yan[3], Yanni Zhao[4], Haolan Zhang[5]

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## Abstract

In this work, the uniaxial hot compression tests of SLM 718 alloy with different orientations were carried out by thermal simulation tester, and the microstructure of the samples before and after deformation was analyzed by scanning electron microscope (SEM) and electron backscattered diffraction (EBSD) technologies. The results show that the orientation of the sample has little effect on the variation of flow stress with strain, but has certain effect on the peak stress. The constitutive equation could accurately predict the hot deformation behavior of the two orientations samples, and the calculated activation energies (Q) of the H-orientation and V-orientation samples are 517.07 kJ/mol and 543.77 kJ/mol, respectively. The analysis of microstructure shows that the dynamic recrystallization (DRX) volume fraction and DRX grain size of the H-orientation samples are higher than those of the V-orientation sample at the same deformation conditions. The DRX mechanism of the two orientations samples is mainly discontinuous dynamic recrystallization (DDRX) and supplemented by continuous dynamic recrystallization (CDRX).

*Keywords: SLM 718 alloy; Compression direction; Flow behavior; Microstructure evolution.*

# A Simple Detection Method of Microdefects during Metal Additive Manufacturing Process Using Acoustic Emission Monitoring

**Kaita Ito**[1], Masahiro Kusano[2], Makoto Watanabe[2], Takayuki Shiraiwa[3], Manabu Enoki[3]

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## Abstract

In laser powder bed fusion (LPBF) additive manufacturing, the powdery metallic material repeatedly melts and solidifies, causing micro-defects. However, it is difficult to detect them by X-ray CT or cross-sectional observation after fabrication because LPBF is generally used to fabricate a large variety of components with complex shapes in small quantities.

We have developed a method to detect generation of microcracks and porosities by acoustic emission (AE) monitoring during LPBF process. The method is practical, simple, and provides location of micro-defects in real time. The most AE events were experimentally confirmed to occur simultaneously with laser irradiation. In other words, the laser irradiation position at the time of AE occurrence can be regarded as the location of microdefects. This relationship was confirmed for several nickel-based superalloy materials and titanium alloys. Therefore, this method can be used independently of the material, size, and shape complexity of the molding object.

Modification of the LPBF equipment by running a cable through the chamber is not easily accepted at the introduction stage of AE measurement. Therefore, we has developed a small wireless AE measurement device. However, since wireless measurement has problems with continuous measurement time limited by battery capacity, and stability of wireless transmission, it is advantageous to introduce wired measurement with minimal chamber modification if AE measurement is to be performed on a permanent basis.

*Keywords: laser powder bed fusion; crack detection; acoustic emission; real-time monitoring*

# Development of Low-Cost Ti-6Al-4V Filler Wire Manufacturing Process for Wire Arc Additive Manufacturing

A.K. Maurya[1,2], N.S. Reddy[2], Seung Won Kang[1], Jae Ho Kim[1],
Jun-ha Yang[1], Jae H. Kim[1], Jong-Taek Yeom[1]*

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[2]School of Materials Science and Engineering, Gyeongsang National University, Jinju, 52828, South Korea.



## Abstract

Recently, WAAM has been in the spotlight as a process that can manufacture large industrial structures quickly and economically. However, the price of filler wire, which is used as a feedstock for WAAM, is still a major obstacle to utilizing this process. Therefore, this study attempted to develop the processing route to manufacture the wire using as cast or β forged Ti-6Al-4V billet bars to reduce the cost of the wire by minimizing processing steps. The hot deformation characteristics of as cast and β forged Ti-6Al-4V have been investigated using thermal-mechanical simulator gleeble-3800 in the temperature range of 700 °C – 1200 °C and strain rate range of $0.01s^{-1}$ – $10s^{-1}$ up to height reduction of 50%. An artificial neural network (ANN) model has been developed to correct the non-isothermal flow stress caused by adiabatic heating. The model-corrected flow stress values were used to construct the processing map at the true strain of 0.6. The microstructural characterization was carried out based on the low and high-efficiency regions of the processing map. The optimum deformation condition of the processing map is further used for hot rolling of as-cast and β forged Ti-6Al-4V billet bar. The developed Ti-6Al-4V filler wire was utilized in the WAAM to analyze the microstructure and mechanical properties.

**Keywords:** Low cost filler wire; WAAM; Ti-6Al-4V; Hot deformation behavior; Artificial neural network;

# A multi-scale numerical and experimental study for solidification microstructure and defects of superalloys fabricated by selective laser melting additive manufacturing

Ling Shi[1], **Songzhe Xu[1]***, Jingjing Li[1], Chaoyue Chen[1], Tao Hu[1], Hari Sundar[2], Jiang Wang[1]*, Zhongming Ren[1]

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## Abstract

A multi-scale model of additive manufacturing process for IN718 alloy is developed based on phase field, automata cellular method and lattice Boltzmann method. For macro-scale, a modified automata cellular method (VISCA) and shan-chen lattice Boltzmann method are fully coupled to compute the powder melting, molten pool flow, and grain growth and investigate the solidification structure and pore defects of multi-layer additive manufacturing. The crystal orientation distribution and pore defects are experimentally observed by EBSD and SEM for the validation of macro-scale model. For meso-scale, a location on the molten pool boundary is simulated based on the crystal orientation, temperature gradient and solidification velocity solved by the macro-scale model to investigate the dendritic growth and laves phase formation using phase field model. The solidification microstructure and laves phase distribution are also experimentally observed by SEM to validate the meso-scale model.

*Keywords: Additive manufacturing; Cellular Automata method; Lattice Boltzmann method; Phase field method; Solidification microstructure; Solidification defects*

# Technical **Oral Session _ Session 8**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 8-2 (E8-2)** **14:00 - 15:30, Nov. 22**

**Chair :** Makoto WATANABE (National Institute for Materials Science) 201B, 2F

14:00-14:15 **O-E0195** **Data assimilation-integrated multi-phase-field simulation of solidification in SUS316L stainless steel during additive manufacturing**
Shoichiro Nakamura (Tokyo Univercity of Agriculture and Technology, Japan)
Johnson Jacob (CSIRO – Commonwealth Scientific And Industrial Research Organization, Australia)

14:15-14:30 **O-E0425** **Development of bio-high entropy alloys (BioHEAs) via laser-powder bed fusion**
Ryosuke Ozasa (Osaka University, Japan)

14:30-14:45 **O-E0910** **Effects of AlN addition on melt pool stability and microstructural evolution of additively manufactured AISI 316L by laser powder bed fusion**
Jung-Wook Cho (Pohang University of Science And Technology, Korea)

14:45-15:00 **O-E1107** **Effect of electropulsing on anisotropy of laser additive manufactured Ti6Al4V alloy**
Wang Fubin (Harbin Engineering University, China)

15:00-15:15 **O-E0751** **Material Extrusion and Photopolymerization Approaches for 3D Printing of Particle-Based Double Network Hydrogels**
Yosuke Watanabe (Yamagata University, Japan)

15:15-15:30 **O-E0608** **Process parameter optimization for the β-solidifying γ-TiAl alloy fabricated by laser powder bed fusion: Evaluation of microstructural and mechanical properties**
Sung-hyun Park (Osaka University, Japan)

# Data assimilation-integrated multi-phase-field simulation of solidification in SUS316L stainless steel during additive manufacturing

**Shoichiro Nakamura**[1], Masahito Segawa[2], Akinori Yamanaka[3]

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## Abstract

A microstructure solidified in additive manufacturing (AM) process is formed under non-equilibrium conditions such as high cooling rate and large thermal gradient. The authors have applied the non-equilibrium multi-phase-field (NEMPF) model coupled with the CALPHAD-based thermodynamic database to simulate the solidification behaviours in SUS316L stainless steel during the AM. The NEMPF model describes the evolution of microstructure and the partitioning of solute atoms at the solid-liquid interface in the non-equilibrium condition. However, the NEMPF model requires material parameters which are difficult to be identified and largely unknown. To solve these issues, data assimilations (DA) are effective because DA can estimate unknown material parameters and unobservable states through integration of simulation results and experimental data. In this study, we develop a new simulation methodology that couples the Bayesian DA with the NEMPF simulation of solidification in Fe-C-Cr-Mn-Mo-Ni alloys during the powder bed fusion AM process. The numerical experiments called twin experiments are performed to validate the estimation accuracy of solidification state and material parameters obtained by the proposed method. The results of twin experiments show that DA can accurately estimate the solidification state and material parameters (e.g., interfacial energy). In order to obtain the accurate DA results, we reduce the computational cost of the NEMPF simulation by replacing the CALPHAD-based thermodynamic database coupling calculation with the machine learning method where the neural network estimates the Gibbs free energy and chemical potential from temperature and chemical composition at the solid-liquid interface region.

*Keywords: Solidification, Additive manufacturing, Multi-phase-field method, CALPHAD, Data assimilation.*

# Development of bio-high entropy alloys (BioHEAs) via laser-powder bed fusion

**Ryosuke Ozasa**[1], Takuya Ishimoto[2], Ozkan Gokcekaya[3], Aira Matsugaki[4], Takayoshi Nakano[5]

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## Abstract

High entropy alloys for biomedical application (BioHEAs) are attracting attention as next-generation biomaterials due to their exceptional mechanical properties and biocompatibility; however, casting, which is a commonly used method for HEA fabrication, results in severe component segregation at slow cooling rates and lacks shape customizability. In this context, this study demonstrates the superior potential of laser power bed fusion (L-PBF) in overcoming these issues by enabling simultaneous suppression of elemental segregation through supercooling, shape customization, and control of crystallographic texture. This study designed the non-equiatomic BioHEAs using empirical parameters and thermodynamic calculations and applied L-PBF, which enables to create a directional and a rapid cooling temperature field, as material creation method. The results showed that the BioHEAs manufactured through L-PBF suppressed phase separation and elemental segregation which is observed in BioHEAs manufactured by arc melting. Crystallographic texture was changed according to the composition of BioHEAs; bimodal texture with fine grain and columnar grain was shown in TiZrNbTaMo-BioHEA, while single crystalline-like texture was shown in TiZrHfNbTaMo-BioHEA. Both BioHEAs showed an excellent combination of strength and biocompatibility. Moreover, single crystalline-like TiZrHfNbTaMo-BioHEA achieved relatively low Young's modulus due to its preferential orientation of <001> along the building direction of L-PBF process. These results suggests that L-PBF process has a benefit to develop functional BioHEAs with less segregation and well-controlled texture.

*Keywords: Bio-high entropy alloys (BioHEAs), Alloy design, Elemental segregation, Laser-powder bed fusion, Crystallographic texture*

# Effects of AlN addition on melt pool stability and microstructural evolution of additively manufactured AISI 316L by laser powder bed fusion

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## Abstract

The AISI 316L stainless steel with the modification of deoxidizer was manufactured by laser powder bed fusion (L-PBF) using 316L powder mixed that included 1 wt% aluminum nitride (AlN) and compared with the as built 316L stainless steel that was manufactured using 316L powder only. AlN addition diminished the oxygen content from 489 ppm (powder) to 244 ppm (316L+AlN), whereas it increased the nitrogen content from 774 ppm (powder) to 1290 ppm (316L+AlN). Reduction behavior was faster in 316L+AlN than in 316L. Larger epitaxial grains were observed from 316L+AlN than 316L within the different textural orientations between two different sets, which correlated to the melt pool's shape and temperature distribution. The inclusions of 316L+AlN were detected as alumina, not nitride, which means nitride was supersaturated. Improvement in the strength of 316L+AlN was measured considering Orowan strengthening, Hall-Petch equation, and dislocation density.

*Keywords: Laser powder bed fusion, Melt pool reduction, Inclusion characteristics, Marangoni effects.*

# Effect of electropulsing on anisotropy of laser additive manufactured Ti6Al4V alloy

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## Abstract

The large temperature gradient during laser metal deposition usually leads to the prior coarse β phase with preferred grain orientation in Ti6Al4V alloy. The phase transition from β to α satisfying the Burgers relationship ultimately produces <$\bar{1}2\bar{1}0$> fiber texture along building direction and the $(01\bar{1}2)$ $[01\bar{1}1]$ plate texture, which directly results in mechanical anisotropy of as-built alloy. In present work, electropulsing was used to treat laser metal deposited Ti6Al4V alloy. The results showed that proper electropulsing treatment leaded to the globularization of α lath and weakened the texture for as-built alloy. The samples deformed along the laser scanning and building directions showed the almost equivalent distribution of Schmid factor and the mechanical anisotropy was reduced from 6.5% to 1.5%. The elongation was significant increased accompanied by a small reduction in yield strength. The present finding provides an effective way to tailor preferred orientations of alloy produced by additive manufacturing.

*Keywords:* materials science, laser metal deposited, electropulsing, titanium alloy, texture

# Material Extrusion and Photopolymerization Approaches for 3D Printing of Particle-Based Double Network Hydrogels

**Yosuke Watanabe[1],** Tatsuya Kobayashi[2], Izumi Ichimori[3],
Jun Ogawa[4], Hidemitsu Furukawa[5]

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## Abstract

Additive manufacturing (AM) is a relatively new research area, similar to research of polymer gels, which can produce geometrically complex customized products with less material and less waste. AM has the ability to create parts directly from digital models in one step. The democratisation of AM technologies, brought about by the open-source 3D printers, is likely to enable more advanced types of co-creation. It is expected that new value will be created in society by the fusion of AM technologies and research of polymer gels.

We have endeavored to develop distinct open-source 3D gel printers, each embracing various approaches such as material extrusion and photopolymerization, for instance, to enable the fabrication of hydrogels with varying degrees of hardness. These 3D gel printers are named “GelPiPer” as the co-creation platform of polymer gels. The term GelPiPer describes the pipeline for polymer gels, indicating that polymer gels are instantly available when the user turns on the GelPiPer.

In this study, we present the findings of the comparative analysis between GelPiPer of material extrusion and photopolymerization, utilizing the particle-based double network (P-DN) hydrogels. To investigate the range of viscosities covered by each approach, we prepared the diverse set of P-DN hydrogel inks, as the viscosity of P-DN hydrogel inks depends on the ratio of the 1st gel powder to the 2nd gel solution. In the material extrusion, the 1st powder plays a crucial role in both thixotropic behavior and post-extrusion shape retention, thereby influencing the fabrication precision.

*Keywords: 3D printer, Hydrogel, Additive manufacturing, Particle Double Network Gel*

# Process parameter optimization for the β-solidifying γ-TiAl alloy fabricated by laser powder bed fusion: Evaluation of microstructural and mechanical properties

**Sung-Hyun Park**[1], Ozkan Gokcekaya[1,2], Ryosuke Ozasa[1,2], Takuya Ishimoto[1,2,3], Ken Cho[1,2], Hiroyuki Y. Yasuda[1,2], Young-Won Kim[4], Myung-Hoon Oh[5], Takayoshi Nakano[1,2,*]

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## Abstract

This study investigates the effect of process parameters on the microstructural characteristics of β-solidifying γ-TiAl alloy fabricated by a laser powder bed fusion (L-PBF) process.

The densification of the L-PBF specimens was altered due to the high crack susceptibility and intrinsic brittleness of intermetallic compounds, however, optimized L-PBF process parameters promised high relative density and defect-free γ-TiAl fabrication.

Especially, variation in the input energy density determined the distinguishable two types of microstructures, which are resulting from the complex thermal history of the L-PBF process. A strong crystallographic texture was observed in the primary β phase at high energy density conditions. In addition, despite the existence of twelve possibilities of α($\alpha_2$) variants from the one parent β phase according to the crystal symmetry, the variant is not randomly selected and the subsequent heat treatment form $\alpha_2/\gamma$ lamellar microstructure followed by Blackburn orientation relationship. On the other hand, the low energy density conditions induce the randomly distributed crystallographic texture in the $\alpha_2$ phase because of the extremely fast cooling rates of the L-PBF process. The microstructure evolution procedure is explained with numerical simulated thermal history. Furthermore, the evaluated mechanical properties of high-densification samples represented a competitive level in comparison with that produced by the traditional method. It means that our research could be the guide reference in the L-PBF process for tailoring microstructures and demonstrates its potential to extend the practical application of β-solidifying γ-TiAl alloy.

*Keywords: Laser powder bed fusion, Titanium aluminide, Microstructure, Mechanical properties*

# Technical **Oral Session _ Session 8**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 8 (F8)** **14:00 - 15:30, Nov. 22**

**Chair :** Soo-Hyun Kim (Ulsan National Institute of Science and Technology) 202A, 2F
Jianhua Yao (Zhejiang University of Technology)

14:00-14:30 **K-F0759** **[Keynote] A patient-centric framework for developing safer 3D printed personalised medical implants**
Peter Vee Sin Lee (University of Melbourne, Australia)

14:30-14:50 **I-F0685** **[Invited] Micro-nano hierarchical metal surfaces for high-performance biomedical applications**
Tingting Song (RMIT University, Australia)

14:50-15:10 **I-F0785** **[Invited] Additive manufacturing of corrosion and wear resistant steel**
Qiyang Tan (The University of Queensland, Australia)

15:10-15:30 **I-F0621** **[Invited] Surface modification of laser deposited materials through ball burnishing**
Anthony Roccisano (University of South Australia, Australia)

# A patient-centric framework for developing safer 3D printed personalised medical implants

**Peter VS Lee**
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## Abstract

Advances in computer-aided engineering, additive manufacturing, and antibacterial coatings have transformed patients' treatment through personalised solutions in orthopaedics and maxillofacial surgery. However, there are significant challenges to facilitating personalised medical implant commercialisation and widespread use. Regulatory frameworks for personalised implants are in their early stages. Current standards for testing off-the-shelf devices are not directly transferrable to devices designed for individual patients. Instead, future test standards could be based on information from the patient's own anatomy and even lifestyle. For example, modifying the surface or structure of load bearing implants without thoroughly understanding the patient's biomechanical loading could lead to adverse outcomes. Successful treatment, therefore, requires a comprehensive approach to optimise the use of the personalised medical device. This presentation will focus on developing a seamless framework based on the Measure-Model-Manufacture-Manage (4M) for point-of-care manufacturing. Comprehensive biomechanical measurements will be used to build patient-specific biomechanical models to represent the underlying physiology of the human body. The models will be used to analyse scenarios that are too expensive or not feasible to perform on patients directly (e.g. loading an implant to failure in the human body). The measure-model stage aims to optimise implant design that considers all the biomechanical information before manufacturing using 3D printing. Finally, the measure-model-manufacture becomes a reinforcing loop that improves patient management and outcome. The presentation will also discuss our experience and benefits, from a researcher's perspective, working closely with physicians, industry, and government leaders in pushing the frontiers of personalised medical implants.

*Keywords : Additive Manufacturing, Medical Devices, Biomechanics, Personalised Implants, Computational Modelling*

# Micro-nano hierarchical metal surfaces for high-performance biomedical applications

**Tingting Song[1]**

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**Abstract**

Conventional copper (Cu) metal surfaces are well-recognized for their bactericidal properties. However, their slow bacteria-killing potency has historically excluded them as a rapid bactericidal material. This work focuses on the development of robust bulk superhydrophilic micro-nano hierarchical Cu surfaces that possess exceptional bactericidal efficacy. It resulted in a 4.41 log10 reduction (>99.99%) of the deadly *Staphylococcus aureus* (*S. aureus*) bacteria within 2 min vs. a 1.49 log10 reduction (96.75%) after 240 min on common Cu surfaces. The adhered cells exhibited extensive blebbing, loss of structural integrity and leakage of vital intracellular material, demonstrating the rapid efficacy of the micro-nano Cu structure in destructing bacteria membrane integrity. The mechanism was attributed to the synergistic degradation of the cell envelope through enhanced release and, therefore, uptake of the cytotoxic Cu ions and the adhesion-driven mechanical strain due to its rapid ultimate superhydrophilicity (contact angle drops to 0° in 0.18 s). The scalable fabrication of these micro-nano Cu surfaces was enabled by integrating bespoke precursor alloy design with microstructure preconditioning for dealloying and demonstrated on 2000 $mm^2$ Cu surfaces.

This development not only paves the way to the practical exploitation of Cu as a low-cost antibiotic-free fast bactericidal surface but also provides a potential pathway for future high-performance hierarchical metal surfaces. A micro-nano hierarchical Ta surface is an immediate example to boot the biocompatibility of conventional Ta implants.

*Keywords: Hierarchical, Metal surfaces, Antimicrobial, Biocompatibility, Dealloying*

# Additive manufacturing of corrosion and wear resistant steel

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## Abstract

Additive manufacturing (AM) has emerged as a transformative technology in the production of advanced engineering metallic materials by offering rapid fabrication with a high design freedom for part complexity and development of new materials through processing the mixtures of different powder feedstocks. In the present work, a powder mixture that consists of AISI 410 and AISI 440 stainless steel powders were prepared and processed with AM. The newly developed steel possessed superior hardness and wear resistance compared to both of the AISI 410 and AISI 440 steels, and most of the commercialized tool steels. The substantial improvement in the wear resistance is attributed to the formation of high-fractions of martensite and carbide nanoparticles within the steel. On the other hand, the corrosion resistance of this steel remained satisfactory, comparable to majority of the martensite stainless steels. This work can be considered as a breakthrough in research of new alloy development using AM.

*Keywords: steels, additive manufacturing, wear resistance, corrosion resistance, SEM.*

# Surface modification of laser deposited materials through ball burnishing

**Anthony Roccisano[1,2]**, Gustavo Fernandez[3,4], Mohammad Uddin[4], Colin Hall[1].

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**Abstract (250 words max)**

Laser metal deposition (LMD) is an industry standard process used for the application of wear and corrosion resistant coatings on metallic substrates as well as the development of additively manufactured features. Whilst some applications allow these materials to be used in the as-deposited state, the vast majority require additional finishing procedures after manufacturing. Improving such properties as surface roughness, hardness, microporosity and microcracks is often required. One method proposed to counter these detrimental defects is ball burnishing (BB), which utilises a rotating ball under pressure to plastically deform the surface for improved material properties. In this study, laser deposited materials were ground and subsequently ball burnished to investigate the impact on the surface properties.

By inducing plastic deformation and dislocation movement, the ball burnishing increased surface and sub-surface hardness of the cladded coating. Further, through the act of ball burnishing the presence of voids and micropores at the surface was diminished, leading to improved sliding wear resistance and corrosion resistance. The surface finish of the laser deposited material was improved through ball burnishing with certain strategies. Most interestingly, when burnishing some materials perpendicular to their direction of deposition, the surface roughness worsened and accentuated the anisotropy of the deposited material. Care must be taken when planning ball burnishing on AM parts that sub-surface anisotropy doesn't lead to poor results.

By leveraging appropriate load and application strategy, ball burnishing can refine the microstructure and surface topography of the coatings leading to enhanced performance of LMD deposited materials.

*Keywords: DED, LMD, ball burnishing,*

# Technical **Oral Session _ Session 8**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 8 (G8)** **14:00 - 15:20, Nov. 22**

**Chair :** Dong-Hwa Seo (Korea Advanced Institute of Science and Technology) 303A, 3F

14:00-14:20 **I-G0420** **[Invited] Ammonia Synthesis via Chemical Looping of Li based Materials**
Hiroki MIYAOKA (Hiroshima University, Japan)

14:20-14:35 **O-G0073** **Heterostructure of Molybdenum Disulfide Zinc Iron Sulfide Hybrid as High Capacity and Long Life Anode Materials for Lithium Ion Batteries**
Jagadis Gautam (Kumoh National Institute of Technology, Korea)

14:35-14:50 **O-G0389** **High-Performance Anode Materials for Sodium/Potassium Ion Batteries**
Chuncheng Yang (Jilin University, China)

14:50-15:05 **O-G0845** **In-situ construction of array structured Bi/N-CNS composite as high-performance sodium-ion battery anode**
Jian Hui Jia (Jilin University, China)

15:05-15:20 **O-G0288** **Phase Field Simulation for Defluoridation of CuPb2F6 Electrode Material**
Iikubo Satoshi (Kyushu University, Japan)

# Ammonia Synthesis via Chemical Looping of Li based Materials

**Hiroki Miyaoka**[1], Shougo Matsumoto[2], Hitoshi Saima[3], Takayuki Ichikawa[4]

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## Abstract

Ammonia ($NH_3$) is recently recognized as an attractive energy or hydrogen carrier to effectively store and transport renewable energy. In this work, the $NH_3$ synthesis processes by chemical looping using Lithium (Li) based materials such as Li alloys and lithium hydride (LiH) are studied. The relationship between reactivity with $N_2$ and the chemical state of Li in the compounds is investigated. From the results, correlation between the reaction temperature and metallic feature of Li in the compounds is clarified [1]. The chemical looping process of Li alloys is composed of 3 step reactions, which are $N_2$ dissociation to form $Li_3N$, $NH_3$ synthesis by reaction between $Li_3N$ and $H_2$, and regeneration of initial alloys from LiH. By all the alloys, $NH_3$ can be synthesized under around 0.1 MPa below 500 °C by gas-switching process. In the case of LiH, $NH_3$ is synthesized by 2 step reactions under $N_2$ and $H_2$, respectively [2]. The reaction kinetics of the chemical looping process by LiH is poor due to the agglomeration of intermediate phase during the reaction. As a result, the reaction is not completed even after about 20 h. The reaction kinetics is drastically improved by mixing LiH with scaffolds to prevent the agglomeration, and then the reaction yield is reached to be almost 100% within 20 min.

This work is supported Grant-in-Aid for Scientific Research (B), JP20H02465 subsidized by JSPS and a project, JPNP2004, subsidized by the New Energy and Industrial Technology Development Organization (NEDO). We would like to thank Research Center for Nitrogen Recycling Energy Carrier at Hiroshima University.

## References

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[2] K. Tagawa, H. Gi, K. Shinzato, H. Miyaoka, and T. Ichikawa, J. Phys. Chem. C, 126 (2022) 2403–2409.

*Keywords: Ammonia, Chemical looping, Lithium compounds, Alloys, Hydrides*

# Heterostructure of Molybdenum Disulfide Zinc Iron Sulfide Hybrid as High Capacity and Long Life Anode Materials for Lithium Ion Batteries

**Jagadis Gautam**[1,2], Dae Heon Kim[1, 2], Kyeong Jun Park[1, 2], Mu Hyeong Kim[1, 2], Jang Seok Gwon[1,2], Mikiyas Mekete Meshesha[1,2], Debabrata Chanda[1,2], Bee Lyong Yang[1,2*]

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**Abstract**

Engineering electrodes with enhanced lithium storage capability and cycling stability is essential for further improving the performance of lithium-ion batteries. In this study, a heterostructure of molybdenum disulfide and zinc–iron sulfide ($MoS_2$@ZnFeS) was synthesized using a two-step hydrothermal method. Morphological characterization of the resulting hybrid material revealed nanosheet-like structures with abundant buffer zones and electroactive centers. The anodic investigation of the hybrid for lithium-ion battery (LIB) applications exhibited an ultrahigh reversible capacity of 685.3 mA h $g^{-1}$ (after 200 cycles at 0.1 A $g^{-1}$), excellent capacity retention (0.017% capacity decay per cycle at 1 A $g^{-1}$ over 1000 cycles), and high rate capability (221.1 mA h $g^{-1}$ at 2 A $g^{-1}$). The impressive Li-storage ability of the hybrid is attributed to the presence of a plentiful buffer zone for volume expansion, a high electroactive surface area, and an abundant of ion exchange pathways. These results demonstrate the benefits of heterostructures of $MoS_2$ and ZnFeS for energy devices.

**Keywords:** Molybdenum disulfide, zinc iron sulfide, anode, lithium-ion batteries

References

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# High-Performance Anode Materials for Sodium/Potassium Ion Batteries

**Chuncheng Yang**[1,*], Q. Jiang[2]

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**Abstract**
Clean and efficient energy storage devices play a vital role in confronting the problems of global warming and energy crisis. Sodium/potassium ion batteries (SIBs/PIBs) have been regarded as the promising alternatives to lithium ion batteries (LIBs), especially in the large-scale energy storage systems, owing to the abundant resource, low cost, environmental friendliness, as well as the similar energy storage mechanism to LIBs. However, the large $Na^+/K^+$ radii bring huge volume change and sluggish kinetics during the charging/discharging processes, and thus poor rate capability and inferior cycling stability. Recently, we proposed a "4S" strategy, *i.e.*, selection, structure, system and synergism. Following this strategy, a variety of anode materials for SIBs/PIBs with excellent rate performance and cycling stability have been developed. Here, two examples are introduced: (i) the hybrid of ultra-small Sb nanoparticles encapsulated in N-doped carbon nanonecklace as the anode material for SIBs; and (ii) the hybrid of ball-cactus-like Bi nanospheres embedded in N-riched carbon nanonetworks as the anode material for PIBs, both of which show excellent electrochemical performances. The proposed strategy provides new ideas to rationally develop high-efficiency and cost-effective anode materials for SIBs/PIBs.

*Keywords: Sodium ion batteries; Potassium ion batteries; Hybrid anode; Electrochemical performance; Structure design*

# In-situ construction of array structured Bi/N-CNS composite as high-performance sodium-ion battery anode

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## Abstract

Sodium ion batteries (SIBs) are considered as one of the most promising energy storage options in the post-lithium era, given the abundant sodium reserves and low cost. However, the rate capability, cycling performance of SIBs have not yet met the requirements of practical applications due to the lack of high-performance anode materials. Bi has recently emerged as an attractive anode material with high capacity and suitable operating potential. Unfortunately, its electrochemical performance is limited by drastic volume changes. Herein, Bi/N-doped carbon nanosheets (Bi/N-CNS) composite is prepared via a facile solvent evaporation and subsequent calcination process. The composite has an array structure with alternating N-CNS and Bi layers consisting of interconnected Bi nanoparticles. The unique structure provides a continuous three-dimensional conductive network and ensures a fast kinetics and efficient alleviation of stress/strain. The Bi/N-CNS composite delivers outstanding Na-storage performance with an ultralong cycle life of 20000 cycles at a current density of 5 A $g^{-1}$ and prominent rate capability of 92% capacity retention at an ultrahigh current density of 100 A $g^{-1}$.

*Keywords: Energy storage technology, sodium-ion battery, alloy anode, array structure, high-rate performance*

# Phase Field Simulation for Defluoridation of $CuPb_2F_6$ Electrode Material

**Shangping. Zhu**[1], Hiroshi. Akamine[2], Takeshi. Tojigamori[3], Hidenori. Miki[4], Kousuke. Noi[5], and Satoshi. Iikubo[6]

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**Abstract**
The grain growth of the active material Cu as the cathode is a serious issue on fluoride ion batteries. In this study, we have investigated the microstructure evolution of $CuPb_2F_6$ cathode material during the discharge process, with a particular focus on Cu nucleation. To address the decreasing F concentration in the microstructure evolution, we have developed the flamework dealing with continuous concentration variation in the phase-field method. We observe that the simulated microstructure shows Cu nucleation from the solid solution phase, named as FCC-int, and the grain size reaches approximately 100 nm by increasing the nucleation frequency, which agrees well with the experimental results. The simulated microstructure with different discharge rate is consistent with the experimental observations with different current. Furthermore, we have investigated the relationship between the number of nucleation, diffusion coefficients, and Cu grain size, and shows that the grain size decreases with increasing discharge rate, nucleation amount, and diffusion coefficient of F in the FCC-int phase.

*Keywords: Fluoride ion battery, cathode material, discharge process, phase-field model, CALPHAD coupling*

This presentation is based on results obtained from a project, JPNP21006, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

# Technical **Oral Session _ Session 8**

## **Symposium H :** Electronic and Magnetic Materials

**Electronic and Magnetic Materials 8 (H8)** **14:00 - 15:25, Nov. 22**

**Chair :** Takamasa Usami (Osaka University) 303B, 3F

14:00-14:20 **I-H0251** **[Invited] Magnetic interaction between nanoparticles synthesized in the cage protein**
Yu Shiratsuchi (Osaka University, Japan)

14:20-14:40 **I-H1082** **[Invited] Magneto-elastic single crystals with large recoverable strain**
Jingmin Wang (Beihang University, China)

14:40-14:55 **O-H0186** **Microstructure and deformation properties of new Bi-based high temperature solders**
LIU BIN (Hiroshima University, Japan)

14:55-15:10 **O-H0924** **Sn(24-2x)Bi18InxSbx solders designed using a dual-cluster model for eutectics**
Zhuang Li (Dalian University Of Technology, China)

15:10-15:25 **O-H0474** **Synaptic features of ZnO/TaOx memristor for neuro-inspired computing**
Tseung-Yuen Tseng (National Yang Ming Chiao Tung University, Taiwan)

# Magnetic interaction between nanoparticles synthesized in the cage protein

**Yu Shiratsuchi**[1,2,3]

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Superparamagnetic nanoparticles (NPs) bound with biomolecules has been attracted much attention for medical application such as hyperthermia and virus detection. Magnetic NPs encapsulated in the protein cage structure are of particular interest because the protein can directly bind the ligands. Virus-like particle (VLP) has a cage structure composed of proteins. Since VLP can capture the virus by the suitable control of the outer structure, the magnetic-NP incorporated VLP is a promising candidate for the above application. Previously, we successfully synthesized the Co-Pt NPs in *Pyrococcus furiosus* virus-like particles (PfVs) and reported that the synthesized Co-Pt NPs were superparamagnetic at room temperature. In order for the design of the suitable magnetic NPs for the above application, the tuning of the magnetic interaction between NPs is crucial. In this work, developing the previous finding, we investigated the magnetic interaction between Co-Pt NPs by utilizing various magnetization measurement techniques such as AC magnetic susceptibility and remanent magnetization.

To obtain the densely packed nanoparticles, we used the PfV crystal. Dispersed Co-Pt NPs were successfully synthesized in the PfV crystals in maintaining the protein crystal structure. With increasing the synthesized amount of Co-Pt, the Co-Pt NPs were aggregated. Interparticle magnetic interaction changed accompanying with the particle aggregation, which manifests in the Mydosh parameter, the Henkel plot and the $\Delta M$ plot. The results also show that the dipolar interaction is predominant, which can be tuned by the structural parameters such as size, interparticle distance and particle arrangement.

*Keywords: Magnetic nanoparticle, Protein, Virus-like particles, Magnetic interaction*

# Magneto-elastic single crystals with large recoverable strain

**Jingmin Wang,** Yijun Chen, Hui Hua, Qijia Yu, Boying Qiao, Shuoyu Zhao, Chengbao Jiang

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**Abstract**

Magneto-elastic materials, including magnetostrictive materials and magnetic shape memory alloys, can exhibit large recoverable strain under magnetic field and have important applications in devices of actuators, sensors, transducers, etc. Developing high-performance magneto-elastic materials with large strain is of crucial importance for fabricating large-stroke, high-resolution and high-efficiency devices. In this talk, we will introduce our recent work on single crystals of FeGa magnetostrictive alloys and NiCuCoMnGa magnetic shape memory alloys.

Single crystals of FeGa magnetostrictive alloys were grown by controlling the solid-liquid interface. Preferential growth of the single crystals along the <001> direction, which corresponds to the highest magnetostriction, was realized. Uniform magnetostriction of the single crystals was achieved by magnetic domain reconfiguration. As a consequence, high-performance FeGa single crystals with uniform magnetostriction of 300 ppm, reaching the theoretical magnetostriction of FeGa alloys, were successfully prepared. Further, FeGaTb single crystals doped by trace Tb element (0.1at%) were grown. The magnetostriction was increased to 400 ppm by the trace Tb element.

In order to explore magneto-elastic materials with larger recoverable strain, NiCuCoMnGa single crystals undergoing magnetic field-induced martensitic transformation were investigated. Quite large recoverable strain was observed under high magnetic field. This was realized by tailoring the phase transformation and the martensite microstructure. This result opens a possible approach to develop advanced magneto-elastic materials.

*Keywords: magneto-elastic materials; magnetostrictive materials; magnetic shape memory alloys; single crystal; recoverable strain*

# Microstructure and deformation properties of new Bi-based high temperature solders

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## Abstract

Sn-Pb alloys were widely used as solder alloys in the electronics industry due to their low cost and excellent properties. However, Pb was harmful to the natural environment and humans. In recent years, with the large-scale integration and miniaturization of electronic products, operating temperatures have become higher than before. Therefore, high-temperature lead-free solder alloys have become a key technology to improve the reliability and life of electronic devices. Bi is a non-toxic metal with very similar properties to traditional Pb-5Sn solder. It is expected to be an alternative to high-temperature lead-free solder. In this research, a series of new high temperature solder was developed by adding In alloy elements on the basis of Bi-2Ag-0.5Cu. The addition of In had resulted in a finer microstructure, besides the eutectic structure, intermetallic compound (IMC) phase with uniform distribution was also found. In the behaviour of deformation at room temperature, the ultimate tensile strength (UTS) reached about 30MPa. In contrast, UTS of pure Bi and Bi-2Ag-0.5Cu were only 11.8 and 21.2MPa, respectively. The finer microstructure and uniform distribution of IMC phase play a role of strengthening, which improved the strength of alloy. However, the improvement in elongation was not obvious. At 373K, the deformation elongation of alloy increased greatly, exceeding 30%, and the tensile strength decreased slightly. Obvious dimples were found at the fracture, which provides reliable evidence for ductile fracture, and also ensuring the stability of alloy at high temperature.

*Keywords: Bi-based alloy, lead-free solders, high temperature solders, microstructure*

# $Sn_{(24-2x)}Bi_{18}In_xSb_x$ solders designed using a dual-cluster model for eutectics

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## Abstract

Sn-Bi solders suffer from the embrittlement arising from the Bi phase. Minor alloying, using for example Sn and In, is a solution but this has to be carried out within a certain composition unit. Our group previously developed a dual-cluster model for eutectics, which describes a binary eutectic as being composed of two cluster-plus-glue-atom units issued from the two eutectic phases, formulated as [dual clusters](glue atoms), as exemplified by $2\{[Sn\text{-}Sn_{10}]Bi_3Sn_1\} + [Bi\text{-}Bi_6]Bi_5 = Sn_{24}Bi_{18} = Sn_{57.1}Bi_{42.9}$ for $Sn_{57}Bi_{43}$ eutectic. In the present work, $Sn_{(24-2x)}Bi_{18}In_xSb_x$ ($x$ =0, 0.2, 0.4, 0.6, 0.8, 1.0) solder series are designed on the basis of the Sn-Bi eutectic dual-cluster formula, where equimolar In and Sb replace Sn. When $x \leq 0.6$, Sb tends to form $\beta$-SbSn phase while In and remaining Sb are dissolved in $\beta$-Sn(Bi) solid solution phase, and Bi phase is refined, reducing its size from 4 μm to 2 μm compared to the eutectic. Their solidification temperature ranges fall between 135.4 and 148.3°C, only slightly larger than that of the base $Sn_{24}Bi_{18}$ eutectic, 140.6 and 150.7°C. When $x > 0.6$, apart from $\beta$-SbSn and $\beta$-Sn(Bi) phases, Sb and In also form high-melting-point $\alpha$-InSb phase, which significantly expands the solidification ranges to between 132.9 and 149.7°C. Among the designed solders, $Sn_{23.6}Bi_{18}In_{0.2}Sb_{0.2}$ exhibits the best performance in terms of the wetting area on Cu substrate (0.1 $mm^2$ per 10 mg) and shear strength (48.0 MPa and 48.5 MPa respectively before and after aging at 110°C for 240h), to compare with 45.8 MPa and 40.1 MPa of the base eutectic $Sn_{24}Bi_{18}$.

*Keywords: Sn-Bi-In-Sb; lead-free solder; eutectic; cluster-plus-glue-atom model; dual cluster model*

# Synaptic Features of ZnO/TaOx Memristor for Neuro-Inspired Computing

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## Abstract

The emerging memristive synapses exhibit a great potential in neuro-inspired computing, which is a new generation of artificial intelligence. A memristor has an excellent capability due to its exceptional features such as high speed in nanoseconds, high ON/OFF ratio, long retention at high temperature, low power consumption, magnificent endurance, and CMOS compatibility for 3D integration technology. A transparent bilayer ZnO/TaOx memristive synapse is presented in this work. The device shows excellent AC endurance ($10^9$ cycles) and high-temperature retention ($10^4$ s) without any degradation at 100 $^0$C. The device exhibits highly stable repetitive 5130 potentiation(P) and depression(D) epochs with 1.026 M pulses. The multilevel characteristics of the device are achieved by changing the pulse height from 0.7 to 1.1 V for long-term potentiation (LTP) and from -0.9 to -1.3 V for long-term depression (LTD) having gradual conductance change for both P and D cases. The synaptic features such as paired-pulse facilitation (PPF) and spike time-dependent plasticity (STDP) are measured using consecutive AC pulses. These unique features confirm that the synaptic device has excellent capability for the application in the neuro-inspired computing systems.

*Keywords: Synapse, Memristor, Neuromorphic, Bilayer oxide, ZnO.*

# Technical **Oral Session _ Session 8**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 8 (K8)** **14:00 - 15:35, Nov. 22**

**Chair :** To be announced Samda Hall B, 3F

14:00-14:30 **K-K1029** **[Keynote] Linking of static heterogeneity to dynamic heterogeneity in fragile metallic glassformer**
Tetsu Ichitsubo (Tohoku University, Japan)

14:30-15:00 **I-K0846** **[Invited] Definition of high-entropy materials via cluster-plus-glue-atom model**
Chuang Dong (Dalian Jiaotong University, China)

15:00-15:20 **I-K1060** **[Invited] A research on the glass-to-glass transition in a high-entropy metallic glass**
Kefu YAO (Tsinghua University, China)

15:20-15:35 **O-K0470** **Abnormal tension-compression asymmetry in terms of anelasticty and yield strength of amorphous Si**
Yuecun Wang (Xi'an Jiaotong University, China)

# Linking of static heterogeneity to dynamic heterogeneity in fragile metallic glassformer

**Tetsu Ichitsubo[1,2]**

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**Abstract**

Glasses, unlike crystalline materials, lack periodic atomic arrangements, posing challenges in determining their structures. In 2005, we proposed that fragile metallic glasses exhibit a static heterogeneous structure comprising regions with strongly and weakly bonded regions (SBRs and WBRs), where the latter are closely associated with the local motion of Johari-Goldstein beta relaxation. To investigate the microscopic structure of glasses from an acoustic perspective, we have employed inelastic X-ray scattering (IXS), which enables the measurement of energy and momentum transfer between X-rays and phonons. Using this technique, we have unveiled the spatial inhomogeneity of glass in terms of local elasticity. This elastic inhomogeneity has been supported by various experiments and simulations and has emerged as a crucial factor influencing their physical properties. However, the interplay between complex relaxations, dynamic heterogeneity, and spatial heterogeneity remains unclear.

In this study, we conducted IXS measurements on metallic glass samples that were rapidly quenched at various rates, aiming to explore the impact of structural relaxation on spatial inhomogeneity. By comparing the local sound velocity, which reflects the nanoscopic structure obtained through IXS, with the ultrasound speed representing the macroscopic structure obtained via resonant ultrasound spectroscopy (RUS) or electromagnetic acoustic resonance method (EMAR), we examined the relationship between the two. Our findings demonstrate that during slow cooling, fragile metallic glasses develop structural heterogeneity through dynamic heterogeneity in α relaxation, whereas less fragile (stronger) glasses maintain a relatively homogeneous structure regardless of cooling conditions. Additionally, we will discuss the effects of sub-Tg annealing on structural heterogeneity during the presentation.

*Keywords: Metallic glasses, structure heterogeneity, dynamic heterogeneity, elasticity, fragility*

# High-entropy feature of austenite stainless steels in terms of the cluster-plus-glue-atom model

**Chuang Dong[1]**, Shuang Zhang[2], Qing Wang[3]

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## Abstract

The contents of Cr and Ni in austenite stainless steels are generally quite high, exceeding 25 wt.% in 304 and 316 grades and even more than half in super austenite stainless steels such as 904L. On the other hand, high-entropy alloys are based on multi-principal-element alloying, instead of single-solvent alloying in conventional alloys. The present work applies the cluster-plus-glue-atom model to identify the chemical units as the composition carrier of stainless steels, for the objective of unveiling their high-entropy feature. This model describes the chemical unit of any solid solution in terms of a nearest-neighbour cluster and a few next-neighbour glue atoms, expressed in the cluster formula form as [central atom - 1st neighbour shell](next neighbour glue atoms). After a full survey on existing industrial stainless steels grades of austenite base, it is pointed out that they are all high-entropy alloys, characterized by mixed occupancies in the 1st-neighbour shells, in sharp contrast to common steels whose 1st neighbour shells are occupied only by the single solvent Fe. Such a structural feature leads to a new definition for high-entropy alloys in terms of the cluster-plus-glue-atom model. Further, examples are given to show the chemical unit formulation facilitates the alloy optimization and development.

*Keywords: cluster-plus-glue-atom model; stainless steels; high-entropy alloys; chemical units; cluster formula.*

# A research on the glass-to-glass transition in a high-entropy metallic glass

**Ke-Fu Yao**

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**Abstract**

Understanding the Glass transition behaviour is a chanllenge and longstanding topics in glass materials. It is clear that studying the glass-to-glass transitions could help to gain an in-depth understanding of the glass nature, but it remains difficult to find the metallic glass with significantly different glass states. Here, we demonstrate that an unusual glass-to-glass phase transition from a high-energy glass state of an equiatomic high-entropy metallic glass NbNiZrTiCo towards a low-energy glass state during heating, together with an enormous heat release even larger than that of the following crystallization at higher temperature. Dramatic atomic rearrangement with short or medium range ordering is revealed by in-situ synchrotron X-ray diffraction analysis. In addition, this glass-to-glass transition leads to significant improvement in the modulus, hardness, and thermal stability, which could promote their applications. These findings create a new pathway for tuning the glass states and properties, and understanding the glass nature and glass transitions.

*Keywords: metallic glass, high-entropy alloy, glass-to-glass transition, thermal stability*

# Abnormal tension-compression asymmetry in terms of anelasticty and yield strength of amorphous Si

**Yuecun Wang[1],** Lin Tian[2], Jun Ding[1]

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## Abstract

Amorphous Si (a-Si) is one of the most important semiconductors and a classic model material for the fundamental research of disordered matter. A-Si typically exists in the form of a thin film and has a range of prominent applications in photovoltaic cells, diverse sensing, MEMS/NEMS, etc. Mechanical behaviours of a-Si at small scale, which have great impacts on the performance, service lifespan, safety and reliability of devices, are of significant technological and scientific interest. However, the intrinsic mechanical properties of free standing a-Si in terms of its elasticity, yield or fracture strength, and plasticity etc. still remain unclear.

Here by taking advantages of the state-of-the-art quantitative in-situ nanomechanical tests, we reveal an abnormal and unusually pronounced tension-compression asymmetry in submicron-sized a-Si: 1) tensile strength astonishingly exceeds compressive strength by a large margin, which is on the contrary to our common sense; 2) in the nominally elastic regime, tensile samples follow the linear elasticity, while hysteresis loops appear on the compression curves, leading to a significant and tunable anelasticity in a-Si nanowires. Molecular dynamics simulations based on the machine-learning and other empirical interatomic potentials reveal that the asymmetry originates from the normal stress-dependent anisotropic evolution of shear moduli, hence altering the magnitude of the activation energy barrier for the elementary shear event under tension versus compression. This hitherto unheralded asymmetry is expected to hold for materials other than a-Si (for example, a-Ge, and silica glass, etc.). This may be of practical relevance to the utility of small-scale glassy materials in microelectronics and microelectromechanical systems.

*Keywords: Amorphous Si, Tension-compression asymmetry, anelasticity, strength*

# Technical **Oral Session _ Session 8**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 8 (L8)** **14:00 - 15:35, Nov. 22**

**Chair** : Mingfang Qian (Harbin Institute of Technology), Qi An (Harbin Institute of Technology) **202B, 2F**

14:00-14:30 **K-L0983** **[Keynote] Balanced strength-ductility match in GNPs/Al composites**
Xuexi Zhang (Harbin Institute of Technology, China)

14:30-14:50 **I-L1140** **[Invited] Effects of 3D Reinforcement using Metal Filaments on the Toughness and Conductivity of Fibre-reinforced Composites**
Raj Ladani (RMIT University, Australia)

14:50-15:05 **O-L0191** **Effects of Initial Texture on the Microstructures and Mechanical Properties of a Cold-rolled Cu-38Zn Alloy**
Yanshuo Li (Kanazawa University, Japan)

15:05-15:20 **O-L0217** **Effect Of FeGa3 On The Wear Of Ultra High Carbon Steel In Atmospheric Environment**
ROONIE PROTASIUS (School of Engineering, Kyushu University, Japan)

15:20-15:35 **O-L0253** **Quantitative evaluation of stress/magnetic field-induced strains of the Ni-Mn-Ga microparticles driving actuation of laminated composites**
DongKeun Han (Tokyo Institute of Technology, Japan)

# Balanced strength-ductility match in GNPs/Al composites

**Xuexi Zhang**, Jianchao Li, Jiajia Li, Mingfang Qian, Lin Geng

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## Abstract

The difficulty in balancing the structural damage and dispersion of graphene nanoplates (GNPs) during ball milling process has made a great compromise in developing high-performance GNPs/Al composites with a balanced strength-ductility match in large-scale production. Here, we proposed a strategy to inhibit GNPs breakage during the ball milling process by controlling the relative size between GNPs lateral size ($d_{GNPs}$) and Al powder diameter ($d_{Al}$). The fragmentation of GNPs in as-blended powder was reduced due to the buffering effect of Al powders when $d_{Al} > d_{GNPs}$. The defect density of GNPs was affected by the contact area between GNPs and milling balls, which was closely related to $d_{GNPs}$ and $d_{Al}$. The lateral size and defect density of GNPs showed a combined effect on the mechanical properties of GNPs/Al composites. GNPs/Al composites with 5 vol% GNPs exhibited excellent strength-ductility match with ultimate tensile strength (UTS) of 344 MPa and elongation of over 10%.

*Keywords: metal-matrix composites (MMCs); nanocomposites; graphene nanoplatelete (GNP); strengthening and toughening*

# Effects of 3D Reinforcement using Metal Filaments on the Toughness and Conductivity of Fibre-reinforced Composites

**Raj Ladani[1],** Sadaf Abbasi[2], Anil Ravindran[1], Chun Wang[3]

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## Abstract

Through-thickness reinforcements in form of stitching, tufting and z-anchoring have been shown to be very effective at improving the modes I, II and mixed-mode interlaminar fracture toughness of composite materials. In this study, the interlaminar fracture toughness and electrical properties of 3D woven composites reinforced with steel and copper z-filaments are compared with a 2D laminate and 3D woven composite reinforced with z-filament made of continuous carbon fibre tows. Experimental testing and finite element modelling of delamination crack growth reveals that metal z-filaments can promote much greater improvements to the mode I interlaminar fracture toughness compared to carbon z-filament. The steel z-filament increases the mode I delamination resistance by over 50 times, with the fracture toughness value (~28 kJ/m$^2$) being the highest reported value for composite laminates. The 3D woven composite containing steel z-filaments has an exceptionally high mode I toughness due to a strong crack bridging toughening mechanism induced by the steel z-filament. The high strength and ductility of the steel z-filaments cause their pull-out and the formation of a very long crack bridging zone which was found to be more effective at improving the mode I interlaminar fracture toughness compared to carbon filaments. The 3D woven composites containing the metal filaments also has significantly higher through-thickness electrical conductivity compared to the 2D laminates. The magnitude of improvements to the interlaminar fracture toughness and electrical properties by metal z-filaments depends on several factors, including the alloy type, mechanical properties (e.g. tensile strength and ductility), volume fractions, and crack bridging toughening mechanisms.

*Keywords: Composite materials, Orthogonal weaving, Damage tolerance, Finite element analysis, Electrical conductivity.*

# Effects of Initial Texture on the Microstructures and Mechanical Properties of a Cold-rolled Cu-38Zn Alloy

**Yanshuo Li**[1], Norimitsu Koga[2], Cihiro Watanabe[3], Hiromi Miura[4]

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## Abstract

Cu-37.75mass%Zn-0.11mass%Sn alloy plates with sharp <001> or <111> textures along the normal direction were prepared. These two specimens were subjected to unidirectional cold rolling, and the effects of the initial texture on mechanical twinning in the early stage of rolling were investigated. The ratio of twinned grains to whole grains in the <001> textured specimen was significantly higher than that in the <111> one. After 90% cold rolling, the so-called heterogeneous-nano (HN) structure, mainly comprising deformation twin domains, shear bands, and conventional lamellae, was clearly developed in both specimens. Tensile tests of the 90%-rolled specimens showed that the <001> textured specimen had a superior strength-ductility balance than that of the <111> one. The superior mechanical properties of the former specimen were attributed to the higher volume fraction of twin domains than that of the latter. Hence, it can be concluded that the initial texture plays an important role in the formation of the HN structure, improving the mechanical properties through more frequent deformation twinning at the early stage of rolling.

*Keywords: Cu-Zn alloy, mechanical property, heavy cold rolling, texture, deformation twin*

# Effect Of $FeGa_3$ On The Wear Of Ultra High Carbon Steel In Atmospheric Environment

**Roonie Protasius[1]**, Masaki Tanaka[2], Kazuyuki Yagi [3],
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## Abstract

Dry sliding tests were carried out to investigate the wear property of $FeGa_3$ on ultra-high carbon steel (UHCS) in an atmospheric environment. A liquid metal of Ga-In-Sn was prepared on the annealed UHCS surface and heated up in a vacuum chamber to produce 1 $\mu$m and 20 $\mu$m $FeGa_3$ layers. The $FeGa_3$ layer has high porosity, high surface roughness, and high hardness. The average grain size of the layer is approximately 0.1 µm. No liquid metal embrittlement was detected beneath the $FeGa_3$ layer. The UHCS consist of a ferrite grain size of 8 µm average with precipitates of chromium carbide. The presence of chromium carbide particles has been detected in the 20 $\mu$m $FeGa_3$ layer and at the surface beneath both layers which could have hindered the further corrosion of the UHCS and also caused the high porosity of the $FeGa_3$ layer. Wear tests using a ball-on-disk tribometer with WC or SUS ball produced a friction coefficient of approximately 0.3 and 0.4, respectively while the wear scar showed adhesion and abrasion wear mechanisms.

*Keywords: $FeGa_3$, Wear, Liquid Metal, Ultra High Carbon Steel, Corrosion*

| O-L0253 |

# Quantitative evaluation of stress/magnetic field-induced strains of the Ni-Mn-Ga microparticles driving actuation of laminated composites

**DongKeun Han**[1], Wan-Ting Chiu[2], Masaki Tahara[3], Volodymyr Chernenko[4] and Hideki Hosoda[5]

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## Abstract

Recently we have developed laminate composites consisting of the layer of single crystalline (SC) Ni-Mn-Ga particles sandwiched between two thin Cu plates as prototypes of actuators. Under magnetic field of about 1 T they exhibited an out-of-plane stroke with a macro magnetostrain up to 3% which was possible to reset by field or mechanical stress.

In the present work we study the microdeformation behaviour of each of the individual particles contained in the magnetostrain active layer of the aforementioned laminated composites as well as their cyclic behaviour through registration of the composite stroke. For quantitative evaluations of the microstrain values of the particles we have utilized an X-ray micro-computed tomography (micro-CT). Furthermore, it was also important to clarify a laminated composite performance by checking its cyclic behaviour and performing cyclic motions, it is essential to confirming its cyclic strain repeatability. For the evaluations of the cyclic stress/magnetic field-induced recoverable shape deformation behaviours and the quantitative estimations of the deformation of composite a less time-consuming focus – out-of-focus optical microscopy (OM) method was used. The cyclic testing was performed 10 times with a resolution of 1 μm. It was confirmed that laminated actuator exhibited a stability of a maximum magnetic field-driven stroke of about 7 μm. It is worth mentioning that the macromagnetostrains obtained by the analysis of both the micro-CT images and OM images have been in a very good agreement. It was shown that the composite actuator exhibited a high stability in terms of cyclic stress/magnetic field-induced motion.

*Keywords: micro deformation, Ni-Mn-Ga, sandwich-structure, composite, magnetostrain*

# Technical **Oral Session _ Session 8**

## **Symposium M :** Nano Materials and Nano Severe Plastic Deformation

**Nano Materials and Nano Severe Plastic Deformation 8 (M8)** **14:00 - 15:20, Nov. 22**

**Chair :** Zenji Horita (Saga University), Guanyu Deng, (The University of Queensland) **402, 4F**

14:00-14:20 **I-M1089** **[Invited] Grain boundary induced deformation mechanisms in nanocrystalline metals by molecular dynamics simulation**
Liang Zhang (Chongqing University, China)

14:20-14:35 **O-M0813** **Biomolecule-initiated interior hotspots for rapid SERS recognition of infectious diseases**
Soo Hyun Lee (Korea Institute of Materials Science, Korea)

14:35-14:50 **O-M0934** **Residual stress and mechanical properties of H beam with pile up by instrumented indentation test**
So-hyeon Lee (Ulsan National Institute of Science and Technology, Korea)

14:50-15:05 **O-M0981** **Correlation analysis between low temperature impact toughness and microstructure depending on heat treatment of 9% Ni steel**
Younghoon Kim (Ulsan National Institute of Science and Technology, Korea)

15:05-15:20 **O-M1074** **The Design and Mechanism Study of new zero dimensional carbon/nitride quantum dots with high antioxidant activity**
Yan Li (University of Science and Technology Beijing, China)

# Grain boundary induced deformation mechanisms in nanocrystalline metals by molecular dynamics simulation

**Liang Zhang**[1], Yasushi Shibuta[2], ChengLu[3], Xiaoxu Huang[4]

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## Abstract

Nanocrystalline metals exhibit many excellent mechanical properties and their underlying deformation mechanisms have been studying widespread. The well-designed atomistic simulations can predict the mechanical behavior of materials ahead of experiments and provide sufficient information on the atomic scale. The choice of appropriate interatomic potential is one of the main concerns of any atomistic simulation that needs to be seriously considered in order to obtain reliable results. We investigated the mechanical response and the deformation mechanisms of nanocrystalline metals (Al, Cu, Ni) under uniaxial loading by molecular dynamics (MD) simulations with different embedded atom method interatomic potentials. The selection of potential has a significant influence on the simulation result, and the reliability of these potentials was evaluated based on the available experimental data in the literature. In the elastic stage, the stress-strain response and Young's modulus of the simulated samples varied with different potentials. Three independent elastic constants of single crystal model were used to predict the isotropic elastic modulus of the polycrystal sample. In the plastic stage, multiple grain boundary (GB) induced deformation mechanisms were observed, including GB migration, intergranular fracture, dislocation nucleation from GB, and deformation twinning. The generalized stacking fault energies were calculated by MD simulation using different potentials, and their effects on the dislocation nucleation and deformation twinning mechanisms were discussed. This work signifies the important role of GBs play in nanocrystalline metals during plastic deformation and highlights the significance of using the appropriate interatomic potential for a specific simulation problem.

*Keywords: Molecular dynamics; Interatomic potential; Grain boundary; Plastic deformation*

# Biomolecule-initiated interior hotspots for rapid SERS recognition of infectious diseases

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## Abstract

Surface-enhanced Raman spectroscopy (SERS) demonstrates great potential for the validation of chemical and biomedical materials because the energy of light inelastically scattered from substances involves unique molecular information (i.e., vibrational energy states). Electric fields confined in dielectric media (i.e., hotspots) make the generation of fingerprint spectrum with an amplified intensity. In particular, SERS substrates with an enhancement factor of $> 10^6$ allow the detection at a single-molecule level. However, SERS applications are limited in practical fields because i) the complicated vacuum techniques are required to prepare highly periodic nanostructures, ii) the randomly diffused molecules are adsorbed on non-plasmonic regions, and iii) the protein scale is generally much larger than nanoscale hotspots. Therefore, the development of novel hotspot models is strategically required.

Meanwhile, interior hotspots have been suggested to reach beyond the conventional SERS platforms. Using various electrochemical methods (e.g., catalytic reduction, galvanic reaction, and electrodeposition), molecules encapsulated by plasmonic nanostructures can be prepared. The embedded substances have dual functions; i) electric field confinement and ii) target analyte. Because both domains are matched, SERS recognition with sensitivity and accuracy is possible. The participation of molecules to become hotspots also contribute to the expansion of limit-of-detection. In addition, the electrochemical techniques provide the advantages of facileness and rapidity.

In this study, we demonstrated biomolecule-initiated interior hotspots for the SERS diagnoses of respiratory diseases via electrodeposition. The fingerprint spectra were detected without labeling processes. The SERS performance was measured in real-time and simultaneously investigated.

*Keywords: Surface-enhanced Raman spectroscopy; Electrochemistry; Respiratory virus; Biosensing*

# Residual stress and mechanical properties of H beam with pile up by instrumented indentation test

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## Abstract

H beam is a structural steel with H shape and has applications in building and ships. It is required to have high performance for safety, and it is researched for having high strength and toughness. It is produced by hot rolling, quenching and self-tempering process (QST process) for having high performance. However, there is a critical issue that the residual stress is introduced during production processing and the performance is degraded by the residual stress. The residual stress is generated by local volume change of material because of thermal gradient in H beam during the production processing. When H beam has the residual stress, combined stress of external stress and residual stress is applied to the beam. It is difficult to predict the failure of the beam under residual stress. Thus, measurement of residual stress distribution is essential for high performance of H beam. In this study, we investigated pile up by instrumented indentation test for estimating residual stress of hot rolled and QST processed H-beam. We measured mechanical properties and residual stress of each position. The relationship of pile up with residual stress and mechanical properties is investigated.

*Keywords: H beam, QST, residual stress, pile up, indentation test*

| O-M0981 |

# Correlation analysis between low temperature impact toughness and microstructure depending on heat treatment of 9% Ni steel

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## Abstract

Due to reinforcement of environmental energy policies, the demand for alternative energy sources such as liquefied natural gas (LNG) has increased. The material of LNG containers is constantly exposed to low temperature due to its low boiling point (-165°C). Therefore, the material of the containers must maintain good mechanical properties not only at room temperature but also at low temperature. However, when the temperature of the material decreases very low, the ductile-to-brittle transition behavior occurs, causing the material to become brittle. So, ensuring excellent impact toughness in low temperature is crucial. It is well-known that to increase the impact toughness of steel materials, the volume fraction of retained austenite needs to be increased through microstructure control. Consequently, research on controlling microstructure through different heat treatment is actively conducted. Analyzing how the microstructure of the material changes depending on the heat treatment conditions and identifying the factors that affect impact toughness will enable the design of materials with high toughness in low temperature using only heat treatment.

In this study, to analyze the effect of heat treatment on low temperature impact toughness, Charpy V-notch tests were performed on 9% Ni steels prepared at each stage of heat treatment. Microstructure analysis was conducted using a scanning electron microscope (SEM) and electron backscattered diffraction (EBSD) to examine the microstructure. Additionally, nanoindentation was conducted to analyze the hardness distribution, aiming to investigate the correlation between heat treatment, microstructure, and mechanical properties.

*Keywords: 9% Ni steel, lamellarizing heat treatment, nanoindentation*

# The Design and Mechanism Study of new zero dimensional carbon/nitride quantum dots with high antioxidant activity

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## Abstract

Reactive oxygen species (ROS) play an important role in biological metabolism. However, abnormally elevated ROS can induce cancer, inflammation and apoptosis. Therefore, the development of highly effective and biocompatible antioxidants is very important for the prevention and treatment of related diseases. In addition, real-time monitoring of intracellular ROS concentration is helpful to explore the pathological process of ROS related diseases and monitor human health status. Here, new zero dimensional carbon/nitride quantum dots (MQDs) with the antioxidant activity and surface state related fluorescence characteristics have been explored to monitor ROS concentration and reduce ROS to a proper level. This work proposes the design, construction and performance research of cell reactive oxygen species visual monitoring and antioxidant. Combined with DFT theoretical calculation, MQDs with high antioxidant activity were designed and constructed. The relationship between the phase composition and surface structure of MQDs and their fluorescence and antioxidant properties and their internal mechanism were studied. Based on their small size and biological safety, we hope the results based on our work provided guidance for the design and mechanism research of new ROS regulation and content monitoring.

Yan Li wishes to make presentation at PRICM11 in the M topic area- Nano Materials and Nano Severe Plastic Deformation.

*Keywords: zero dimensional carbon/nitride quantum dots, antioxidant, ROS, real-time monitoring*

# Technical **Oral Session _ Session 8**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 8-1 (N8-1) 14:00 - 15:30, Nov. 22**

**Chair :** Hyo-Sun Jang (Korea Institute of Materials Science) 203, 2F

14:00-14:15 **O-N0275** **Molecular dynamics simulation of three-dimensional ferrite nucleation behavior during austenite-to-ferrite transformation in pure iron**
Mizuki Serada (Tokyo University of Agriculture and Technology, Japan)

14:15-14:30 **O-N0919** **Machine learning-based scale-bridging approach for the evolution of irradiation-induced defects in tungsten**
Linyun Liang (Beihang University, China)

14:30-14:45 **O-N0673** **Modeling defect sink mechanism of lath boundary dislocation network using anisotropic linear elasticity method**
Hadi Ghaffarian (KAIST, Korea)

14:45-15:00 **O-N0274** **Development of continuous cluster-activation method and its application to various phenomena in materials science**
Ryo Yamada (Hokkaido Univerisity, Japan)

15:00-15:15 **O-N0525** **Molecular Dynamic Simulation of Primary Damage in High Entropy Alloys: Examining the Interplay of Alloying and Grain Boundary Effects for Superior Irradiation Resistance**
Mosab Banisalman (Virtual Lab Inc, Korea)

15:15-15:30 **O-N0546** **Nuclear quantum effects on hydrogen-isotope diffusion in vanadium and palladium: A path-integral molecular dynamics study**
Hajime Kimizuka (Nagoya University, Japan)

# Molecular dynamics simulation of three-dimensional ferrite nucleation behavior during austenite-to-ferrite transformation in pure iron

**Mizuki Serada**[1], Tomoo Fujiwara[2], Akinori Yamanaka[3]

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## Abstract

Solid phase transformation in steels is an important phenomenon to control the mechanical properties of steels. In particular, the austenite-to-ferrite ($\gamma \rightarrow \alpha$) transformations among the solid phase transformations in steels is essential to determine the morphology of hard microstructures (e.g., martensite phase). However, three-dimensional nucleation behaviour of the $\alpha$ phase during the $\gamma \rightarrow \alpha$ transformation is difficult to observe directly by experimental methods. On the other hand, atomic-scale simulation of the $\gamma \rightarrow \alpha$ transformation using molecular dynamics is effective to investigate nucleation and growth of the $\alpha$ phase in nano-meter length-scale. In this study, we investigate three-dimensional nucleation behaviour of the $\alpha$ phase during the $\gamma \rightarrow \alpha$ transformation in pure iron using molecular dynamics simulations. In particular, three-dimensional nucleation behaviour of the $\alpha$ phase in polycrystalline $\gamma$ phase during isothermal holding process is simulated using various interatomic potentials. The results show that the $\alpha$ phases are nucleated preferentially at the multiple junctions of the $\gamma$ grain boundaries (i.e., corner, edge, and face) as reported by the previous studies. Furthermore, the relationships between the morphology of nucleated $\alpha$ phases and the nucleation site is clarified. The results also reveal the temperature-and $\gamma$ grain size dependency of the preferential nucleation sites and nucleation rate of the $\alpha$ phases.

*Keywords: Molecular dynamics simulation, Austenite-to-ferrite transformation, Steel, Nucleation.*

# Machine learning-based scale-bridging approach for the evolution of irradiation-induced defects in tungsten

**Linyun Liang[1,2]**, Ruihao Liao[1,2], Ke Xu[1,2], Shuo Jin[1,2], Guang-Hong Lu[1,2]

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## Abstract

Irradiation alerts the materials at different scales spanning from atomic processes, and microstructural evolution to macroscopic properties. Many efforts have been made on multiscale simulations to reveal the relation between the atomic structure and the microstructural morphology of the materials. The phase-field method, as a mesoscale diffuse-interface approach, faces challenges in explicitly capturing the nucleation process because the thermal activation process is inherently incompatible with the derivation of the governing equations. The direct utilization of the defect structures obtained from the molecular dynamics method (MD) as the early stages of irradiation defects in the phase-field model is also prevented due to the extremely large computational cost. To this end, we propose an integrated model to bridge the atomic scale to the microstructural scale by developing a machine-learning method. We take the evolution of neutron irradiation-induced voids in tungsten (W) as an example. The displacement cascades at a given energy are first simulated by MD. These results are used to train the machine-learning model to predict the distribution of point defects within the damage energy range of 0-100 keV. Remarkably, it only requires 0.25 seconds to generate a set of defect data at a given energy, which improves the speed by four orders of magnitude compared to MD simulations. The obtained defect structures are subsequently taken as input for the phase-field model to evolve at the diffusion time scale. The integrated model provides an efficient and effective multi-scale simulation approach for understanding and predicting the evolutions of irradiation-induced defects in nuclear materials.

*Keywords: multi-scale, machine learning, irradiation, defect evolutions, tungsten*

# Modeling defect sink mechanism of lath boundary dislocation network using anisotropic linear elasticity method

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## Abstract

Ferritic-Martensitic (FM) steels with hierarchically-arranged microstructure are the leading candidate structural materials for the next generation of nuclear reactors. Lath boundaries (LBs), the primary microstructure unit in FM steels, have a crucial role in the plasticity of these steels. The LBs are made up of a hexagonal dislocations network (HDN) formed by an array of ½<111> screw dislocations lying on the interface. These boundaries also possess a remarkable capacity for defect sinking and can absorb various irradiation-induced defects, such as vacancy clusters and dislocation loops. The sinking mechanism of FM steels is not yet fully understood because of the small size of LBs and the multi-scale complexity of FM steels. Nonetheless, it is widely acknowledged that the sinking mechanism is primarily driven by the interaction between the stress field of the structural defect and the defects induced by irradiation. These interactions can be accurately modeled using the elastic field theory method.

Therefore, this study aims to develop a model for the interaction between the stress field of LBs and those from the Frank dislocation loops and vacancy clusters in bcc Fe. For this goal, we utilize anisotropic linear elasticity to derive the stress field of the corresponding LBs and defects. We then perform a rate theory Monte-Carlo simulation to identify the preferred sinking locations on the LB plane. Our findings indicate that the nodal points on the LB exhibit the greatest potential for defect precipitation as a result of their high localized elastic stress intensity.

*Keywords: Anisotropic linear elasticity, dislocation network, rate theory, defect sink, lath boundary*

# Development of continuous cluster-activation method and its application to various phenomena in materials science

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## Abstract

Atomistic behaviours in metals and alloys have been broadly investigated using molecular dynamics (MD) simulation. The applicability of MD simulation, however, is limited to a phenomenon at relatively small time scale. Recently, phase-field crystal (PFC) method has attracted lots of attentions because it can simulate atomistic behaviours at diffusive time scale. The PFC method is versatile, and a variety of phenomena have been simulated. However, it is basically a phenomenological approach, and a determination of input parameters in PFC method is not an easy task, which limits the applicability. In this work, a new atomistic simulation model is proposed, which is an extension of cluster activation method (CAM) from discrete to continuous spaces (so-called continuous CAM). In this work, a variety of phenomena in a pure metal, such as solidification, nucleation of solid, and grain coarsening, was simulated using continuous CAM, where Lennard-Jones potential was employed for the simplicity. It was confirmed that a quite similar solidified microstructure with PFC method can be produced by continuous CAM. Furthermore, the dependency of grain boundary energy on orientational mismatch between neighbouring grains fits well with the Read-Shockley equation for small misfit orientations. It is noteworthy that the continuous CAM employs interatomic interaction energies as main input parameters, which is in contrast with the fact that the PFC method needs phenomenological input parameters.

Topic area: Computational Materials and Artificial Intelligence

*Keywords: atomistic simulation, diffusive time scale, cluster-activation method*

# Molecular Dynamic Simulation of Primary Damage in High Entropy Alloys: Examining the Interplay of Alloying and Grain Boundary Effects for Superior Radiation Resistance

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**Abstract**

This research delves into the radiation resistance of High Entropy Alloys (HEAs) using comprehensive Molecular Dynamic (MD) simulations, with a particular focus on the nuanced influences of alloying and various grain boundary configurations. An intricate alloy structure was fabricated by selectively substituting Fe, Cr, Co, and Cu atoms with Ni atoms in a 50x50x50 supercell to attain high entropy content. We scrutinized four distinct alloying sets of HEAs, namely, 28Ni, 12Co, 16Co, and 20Ni, characterized by specific atomic ratios of the constituent elements. The aim was to comprehend how these varied compositions influenced the radiation damage resistance. A detailed examination of three different grain boundary configurations further underscored their role in radiation damage mitigation. In our findings, specific grain boundary configurations, notably the second and third, substantially reduced vacancy defects, while the third type significantly diminished self-interstitial atom (SIA) defects. Using a primary knock-on atom (PKA) energy of 100keV, we simulated radiation events and evaluated the resultant defect formations. The investigation extended to the formation of Frenkel pairs and the characterization of emergent interstitial displacement loops, analyzed through the Dislocation Extraction Algorithm (DXA). With these insights, an optimal alloy showcasing robust mechanical properties and radiation resilience was proposed. These comprehensive findings highlight the potential of HEAs for various applications, especially in high-radiation environments, and could direct future research towards developing advanced alloys with enhanced performance attributes.

*Keywords: High Entropy Alloys; Molecular Dynamics Simulation; s Radiation Resistance; Grain Boundary; Alloying Effects.*

*Suggested section:*

*Computational Materials and Artificial Intelligence*
*Or*
*Structural Materials for High Temperature*

# Nuclear quantum effects on hydrogen-isotope diffusion in vanadium and palladium: A path-integral molecular dynamics study

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## Abstract

Measuring the diffusion rate of hydrogen isotopes in metals and alloys is important for understanding isotope effects on the kinetics of hydrogen transport and hydrogen-induced deterioration of materials. However, there is still no consensus on the physical mechanisms for the hydrogen-isotope diffusivity in representative metals. In this study, we investigated the diffusion behavior of interstitial hydrogen isotopes in body-centered cubic (bcc) vanadium and face-centered cubic (fcc) palladium using path-integral centroid molecular dynamics (CMD) method, which approximates the real-time evolution of particles based on quantum statistical mechanics. The diffusion coefficients of hydrogen isotopes were evaluated by calculating the time evolution of the mean-square displacement of hydrogen-isotope atoms in metals at various temperatures. The obtained results were in excellent agreement with experimental measurements over a wide temperature range. By considering the nuclear quantum effects (NQEs), the temperature dependence of the hydrogen diffusivity in vanadium has a "C" shape on Arrhenius plots. This implies that, in the case of bcc metals, the hydrogen diffusivity in the quantum regime is much higher than that in the classical regime. Furthermore, we investigated the hydrogen-isotope diffusivities in fcc palladium over a wide temperature range using path-integral molecular dynamics (PIMD) calculations in the framework of density functional theory-informed artificial neural networks [1,2]. The NQE on the activation free energies for hydrogen-isotope migration was characterized according to the free energy profiles obtained from the thermodynamic integration of the centroid force along the migration path at 75-1200 K. We found that the temperature dependence of the diffusivities in palladium has an unusual "reversed S" shape on Arrhenius plots. This irregular behavior, which stems from the competition between different NQEs with different temperature dependencies, unravels the mechanism of anomalous crossovers between the normal and reversed isotope effects that were experimentally observed.

[1] H. Kimizuka, S. Ogata, and M. Shiga, Phys. Rev. B **100**, 024104 (2019).
[2] H. Kimizuka, B. Thomsen, and M. Shiga, J. Phys. Energy **4**, 034004 (2022).

*Keywords: Hydrogen diffusivity, Nuclear quantum effects, Path-integral simulations, Machine-learning potentials*

# Technical **Oral Session _ Session 8**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 8-2 (N8-2)** **14:00 - 15:30, Nov. 22**

**Chair :** Kyoungdoc Kim (Pohang University of Science and Technology) 400, 4F

14:00-14:15 **O-N0130** **Data assimilation-integrated phase-field simulation of ternary alloy solidification in forced convection using local ensemble transform Kalman filter**
Masahiro Kawasaki (Tokyo University of Agriculture and Technology)

14:15-14:30 **O-N0707** **Phase field study of solid-state sintering process in Fe-Si alloys**
Sandeep Sugathan (Kookmin University, Korea)

14:30-14:45 **O-N0258** **Simulation of microstructural evolution during active metal brazing with Ag-Cu-Sn-Ti alloy by CALPHAD coupled phase-field method**
Takumi Morino (Yokohama National University, Japan)

14:45-15:00 **O-N0462** **Phase Field Modelling of Martensitic Phase Transformation by transient heat transfer**
Dong-Wook Lee (Technology Innovation Institute, UAE)

15:00-15:15 **O-N0141** **Modeling of Crystal Plasticity Predicting Microstructural Changes Caused by Twinning-Induced Plasticity**
Haruki Ohashi (Tohoku University, Japan)

15:15-15:30 **O-N0398** **Material parameter estimation for aluminum alloy sheet using non-sequential data assimilation**
Michihiko Suda (Tokyo University Of Agriculture And Technology, Japan)

# Data assimilation-integrated phase-field simulation of ternary alloy solidification in forced convection using local ensemble transform Kalman filter

**Masahiro Kawasaki**[1], Akinori Yamanaka[2]

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## Abstract

Because the mechanical properties of alloys strongly depend on their microstructure inside the alloy, it is important to understand the dendritic growth of crystals that determines the solidified microstructure formation process. Although direct experimental observations of growing dendritic microstructures (dendrites) have been reported in previous studies, it is difficult to measure the state of solidification, such as solute concentration and flow velocity of the liquid phase from experiments. Therefore, numerical simulations of dendrite growth using the phase-field method have been widely performed. However, many parameters involved in phase-field models of alloy solidification are generally unknown. Our research group has proposed data assimilation methodologies to estimate the unknown parameters of the phase-field model from experimental data. In particular, the previous study applied the local ensemble transform Kalman filter (LETKF), which is one of the most computationally effective methods for sequential data assimilation, to the phase-field simulations of alloy solidification. In this study, this LETKF-based three-dimensional phase-field model (LETKF-PF) is coupled with the Navier-Stokes (NS) equation to calculate the fluid flow, to develop a numerical simulation model (LETKF-QPF-NS) that can be directly compared with experimental data. Furthermore, we perform numerical experiments to validate the estimation of the material parameters and the states including solute concentration, velocity fields and boundary conditions in a Fe-C-Mn alloy. The numerical experiment results demonstrate that the LETKF-QPF-NS model can simultaneously estimate the solute concentration field, velocity field, solute diffusion coefficient, interfacial energy, and inlet flow velocity of boundary conditions only from the morphological data of growing dendrites.

*Keywords: Data assimilation, Phase-field simulation, Computational Fluid Dynamics, Solidification*

# Phase field study of solid-state sintering process in Fe-Si alloys

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## Abstract

Particle sintering is a widely used powder-processing method to fabricate metal and ceramic parts. Sintering induces morphological changes in the green compact, reducing surface area and increasing density. Understanding the mechanisms behind the densification and microstructural evolution during the sintering process is of immense importance because of its broad industrial applications. A phase field model with the relaxation of partition coefficient is developed to describe the microstructural evolution during solid-state sintering in binary alloy systems. In this model, we replace the equal diffusion potential condition using the relaxation equation of the partition coefficient. In the interfacial region, the criterion for the relaxation parameter is modified to maintain the equal diffusion potential condition. The model considers different diffusion mechanisms including volume diffusion, surface diffusion, and grain boundary diffusion together with grain boundary migration. The model is applied to the sintering process with Fe-Si powders, for which the Gibbs energies are modeled based on the CALPHAD database. The model is implemented using parallel GPU computation to simulate the sintering of multiple particles efficiently. We validate the model by matching two-particle sintering simulations with the analytic solutions. We also investigate the relation between the dihedral angles and energy ratios of the sintered powder particles. Furthermore, the results of large-scale sintering simulations of multiple particles are compared with an existing analytic model.

*Keywords: Phase-field model; Sintering; Diffusion; Grain boundary migration.*

# Simulation of microstructural evolution during active metal brazing with Ag-Cu-Sn-Ti alloy by CALPHAD coupled phase-field method

**Takumi Morino**[1], Shoichi Hirosawa[2], Machiko Ode[3], Taichi Abe[3], Yoichiro Mori[4], Seiichi Suenaga[4]

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## Abstract

In active metal brazing process to joint ceramics substrate with copper circuit, it is quite important to clarify solidification behavior of brazing metals by considering the effect of their reactions with ceramics materials (e.g. $Si_3N_4$). Commercially utilized Ag-Cu-Sn-Ti alloy is an example of brazing metals in which the depletion of active Ti occurs as a result of $9Ti+Si_3N_4 \rightarrow 4TiN + Ti_5Si_3$ reaction with $Si_3N_4$ substrate. In this study, CALPHAD database of Ag-Cu-Sn-Ti system has been newly developed by thermodynamic assessment, and then applied to a phase-field program for simulating microstructural evolution during active metal brazing with Ag-Cu-Sn-Ti alloy. The phase-field program of our own coding could successfully investigate the effect of Ti depletion on solidification microstructures and liquidus/solidus temperatures.

From the results of thermodynamic assessment, for example, solidified phases of Ag-Cu-Sn-Ti alloys were predicted to mainly consist of primary $Sn_3Ti_5$ and eutectic Ag and Cu although the amount and solidified temperature of each phase significantly varies depending on cooling rates. The simulated microstructures well depicted such a difference; i.e finer primary $Sn_3Ti_5$ and narrower lamellar spacing of Ag/Cu eutectic with lower solidus temperature in Scheil solidification (faster cooling rate) than those in equilibrium solidification (slowest cooling rate).

From the simulated microstructures by considering the effect of Ti depletion, furthermore, it was found that the decreased amount of primary $Sn_3Ti_5$ increases Sn concentration in Ag-Cu-Sn-Ti alloy liquid, resulting in the lowering of solidus temperature. Such a finding reinforces insights from industrial experience, and thus provides some guidelines for designing Ag-Cu-Sn-Ti alloy brazing.

*Keywords: Phase-field method, CALPHAD, Ag-Cu-Sn-Ti, Active metal brazing, Solidification*

# Phase Field Modelling of Martensitic Phase Transformation by transient heat transfer

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## Abstract

Shape memory alloys have unconventional functionalities which are called shape memory and pseudoelasticity effects originating from martensitic phase transformation. Here we resent phase field simulation of martensitic microstructure evolution based on novel Gibbs potential which correctly describes typical features of SMAs such as constant transformation strain, weakly temperature dependent or constant stress hysteresis, and transformation at nonzero tangent elastic moduli. A finite element method is proposed for modelling of stress- and constant or transient temperature-induced martensitic phase transformation such as cubic to tetragonal, orthorhombic, and monoclinic martensitic phase. This model consists of three coupled equations such as Ginzburg-Landau, elasticity, and heat conduction equations with several initial conditions such as different stresses and temperatures to show the shape memory and pseudoelasticity effects due to martensitic phase transformation. The experimentally observed microstructures such as needle, lamellar, zigzag twins, tapered V-shape twins, and tweed are simulated in this study. Interface direction of these microstructural patterns consistent with a prediction of the crystallographic theory.

*Keywords: Phase Field Method, Martensitic Phase Transformation, Heat Transfer*

# Modeling of Crystal Plasticity Predicting Microstructural Changes Caused by Twinning-Induced Plasticity

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## Abstract

It is well known that the strength and ductility of metals are a trade-off. Recently, it has been reported that the twinning-induced plasticity (TWIP) effect can overcome this trade-off. Twinning deformation accompanies a change of crystal orientation, a local twinning shear, and an increase in dislocation density in the twin phase. These microscopic phenomena are thought to be the fundamental mechanism of the TWIP effect. Controlling the microstructure, for example, grain size and alloy composition, may allow for more effective use of the TWIP effect. However, searching for suitable conditions using experiments will take time and effort. The numerical simulation using the theory representing the TWIP effect consistent with actual phenomena will make efficient the material design. The crystal plasticity theory, which is based on slip deformation, has already been established. Deformation twinning is observed at the grain size scale, so some studies have attempted to extend this theory to the TWIP effect. However, simulations using these models show different results from experiments because of their insufficient assumptions. This study proposes a continuum model based on actual phenomena that can predict the TWIP effect. Local twinning shear is expressed by applying the crystal plasticity theory. Furthermore, the proposed model considers the additional slip deformation to relax the stress caused by the local twinning shear and constraint from surrounding matrices. Numerical simulation based on the proposed model confirms the reproduction of the increase of dislocation density at the twin phase.

*Keywords: Twinning Deformation, Crystal Plasticity, Dislocation Density, Low Stacking Fault Energy Material, Finite Element Method.*

# Material parameter estimation for aluminum alloy sheet using non-sequential data assimilation

**Michihiko Suda**[1], Kengo Sasaki[2, 3], Akimitsu Ishii[4], Sam Coppieters[5] and Akinori Yamanaka[6]

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## Abstract

To reduce the weight of automobiles, it is effective to develop new aluminum alloy sheets which can be applied to automotive components. However, the formability of aluminum alloy sheets is inferior to that of steel sheets. This disadvantage results in wrinkling and cracking in sheet metal forming processes. To solve this problem, finite element method-based sheet metal forming simulation has been used to improve the forming process. In order to improve the prediction accuracy of sheet metal forming simulation, it is necessary to calibrate a yield function and its parameters (i.e., the material model) that accurately describes elastoplastic deformation behavior of aluminum alloy sheets. In previous studies, a multi-axial stress test was used to accurately calibrate the material model. However, to the best of the authors' knowledge, no material modeling method that can simultaneously calibrate the parameters of the material model and the process parameters such as the friction coefficient has been reported. The purpose of this study is to develop a new material modeling method by integrating experimental data into the sheet metal forming simulation with the data assimilation method based on Bayesian inference. In this contribution, we present data assimilation approach to simultaneously calibrate the material model and friction coefficients from full-field strain measurement data obtained by digital image correlation. We demonstrate that the calibrated material model contributes to improving the prediction accuracy of the hole expansion simulation. Furthermore, we validate the robustness of our proposed method by applying the material model to different sheet metal forming simulations (e.g., deep drawing).

*Keywords: Data assimilation, Material modelling, Finite Element Method*

# Technical **Oral Session _ Session 8**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 8 (O8)** 14:00 - 15:05, Nov. 22

Chair : Jae Hong Shin (Korea Institute Of Industrial Technology) 401, 4F

14:00-14:20 **I-O0860** **[Invited] Validating Agar as an Analog of Soil to Monitor Corrosion of Pipeline Steel**
Xiaobo Chen (RMIT University, Australia)

14:20-14:35 **O-O0292** **Machine learning-based localized corrosion prediction considering local microstructural features in AA5083 alloy**
Kaige Wu (The University of Tokyo, Japan)

14:35-14:50 **O-O0331** **Analysis of localized corrosion behavior of Mg89Zn4Y7 alloy through acoustic emission with high-speed microscopic imaging**
Nobu Yatagai (The University of Tokyo, Japan)

14:50-15:05 **O-O0361** **Effects of microstructural factors on corrosion properties of magnesium alloys processed by different wrought processing**
Suda Masataka (Doshisha University, Japan)

# Validating Agar as an Analog of Soil to Monitor Corrosion of Pipeline Steel

**Xiao-Bo Chen**[1], Kai Rui Wang[2], Asma Lamin[3], Amy J. Spark[4], Liam Ward[5], and Ivan Cole[6]

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## Abstract

Aqueous electrolyte traditionally used for electrochemical characterization of soil-related corrosion in laboratories fails to represent the soil physical features, such as pore structure, soil heterogeneity, soil compaction, and saturation levels, in the diffusion-controlled corrosion process. This article introduces a semi-solid agar system to reproduce the physical structure of soil for corrosion study. For feasibility validation of the agar system, direct comparison regarding electrochemical activity, diffusion characteristics, and corrosion mechanisms has been performed on pipeline steel in aqueous sodium chloride (NaCl) solution (5 g $L^{-1}$), 5 g $L^{-1}$ NaCl-containing agar, and 5 g $L^{-1}$ NaCl in sand, respectively. The results indicates that oxygen diffusion in agar and sand media is similar, which significantly weakens the cathodic activity of steel specimens, but leads to distinct corrosion characteristics from those identified in aqueous NaCl solution counterparts. The high diffusion rate of chloride ions in aqueous solution also accelerates corrosion of pipeline steel in NaCl solution through extensive attack at defect sites, but the limited chloride ion movement and the diminished driving force for anodic corrosion activity reduce such attack in their agar and sand equivalents. The solid nature of agar outperforms aqueous electrolytes as soil replicate to explore soil-related corrosion responses at laboratory scale.

*Keywords: Agar, Carbon Steel, Diffusion, Oxygen Reduction, Soil Corrosion*

# Machine learning-based localized corrosion prediction considering local microstructural features in AA5083 alloy

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## Abstract

The localized corrosion behavior of AA5083 alloy has been well known to be largely dependent on the local microstructure, i.e., micro-sized intermetallic compound particles (IMPs). Existing studies have primarily aimed to elucidate the role of iron-rich or magnesium-rich IMPs as cathodic or anodic inclusions compared to the surrounding Al matrix in localized corrosion. However, a statistical study of localized corrosion considering the contribution of various microstructural parameters is still lacking. In this work, a framework based on automated particle analysis, intermittent anodic polarization test, and machine learning approach was proposed to statistically analyze the role of multiple microstructural features, including compositional and geometric parameters, in determining the occurrence and susceptibility of localized corrosion in AA5083 alloy. Prior to corrosion testing, 16 shape features and 10 element features of each IMP on the exposure area were extracted through the SEM-EDS-based particle analysis. In the following, an intermittent anodic polarization (IAP) test was performed to obtain the occurrence and breakdown potential of localized corrosion at the corroded IMPs. Then, a linear support vector machine algorithm was applied to analyze the microstructural features between corroded and non-corroded IMPs. The results showed that the occurrence of localized corrosion could be classified and predicted with an accuracy of 97.2%. In addition, the linear regression analysis of the breakdown potential of corroded IMPs suggested that the smaller the alloying element, area, max length, and Feret diameter of the IMPs, the greater the possibility of localized corrosion.

*Keywords: Pitting corrosion, intermetallics, machine learning, particle analysis, intermittent anodic polarization.*

# Analysis of localized corrosion behavior of $Mg_{89}Zn_4Y_7$ alloy through acoustic emission with high-speed microscopic imaging

**Nobu Yatagai[1]**, Kaige Wu[1], Takayuki Shiraiwa[1], Manabu Enoki[1]

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## Abstract

Mg alloys containing long period stacking ordered (LPSO) phase are receiving a lot of attention because of their excellent mechanical strength. However, the details of their localized corrosion behavior are still unknown. In particular, it is difficult to observe pit initiation because it occurs in extremely small dimensions and super short timescales.

In this study, anodic polarization tests on $Mg_{89}Zn_4Y_7$ alloys in NaCl solution saturated with $Mg(OH)_2$ were performed with in-situ monitoring by high-speed microscopy and acoustic emission (AE) to elucidate local corrosion initiation and propagation behavior. As a result, the first AE signal was detected when there was no visible change on the sample surface, which revealed that the passive film breakdown can produce AE signals. Subsequently, AE signals were continuously detected with a decreasing trend in AE peak frequency during the $H_2$ bubble generation and growth around Y-rich inclusions. Through analyzing the AE signals from a single $H_2$ bubble growing from a few μm to over 100 μm, an inversely proportional relationship was found between the diameter of $H_2$ bubbles and the AE peak frequency. Through an investigation on the cross-sectional morphology of several pits of different conditions, the relationship between the state of the passive film and the feature of the first AE signal was discussed. Furthermore, after clarifying the characteristics of AE signals originating from passive film breakdown, bubble generation and bubble growth, these signals are used as training data to establish a prediction model for localized corrosion phenomena of Mg-Zn-Y alloys.

*Keywords: Mg alloy, LPSO phase, pitting corrosion, hydrogen bubble evolution, acoustic emission.*

# Effects of microstructural factors on corrosion properties of magnesium alloys processed by different wrought processing

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## Abstract

Magnesium alloys are promising materials for light-weighting applications in various industrial fields such as transportation vehicles, and aerospace applications, owing to their low density and their high specific strength, and good recycling properties among practical metals and alloys. However, their widespread applications are still restricted due to their inferior ductility, strength, and especially poor corrosion resistance, compared with aluminum alloys and steels. Although many researchers have investigated the corrosion properties of magnesium alloys, most of the previous studies have reported the corrosion properties of magnesium alloys by one kind of wrought process, and few studies have systematically compared the corrosion properties of magnesium alloys by different wrought processes.
Thus, the purpose of the present study is to systematically investigate the corrosion properties of AZ31 magnesium alloys processed by five different wrought processes (forging, rolling, extrusion, equal-channel-angular-extrusion, and caliber rolling) and evaluate the effects of microstructure factors on corrosion resistance. In this study, we tried to apply machine-learning and statistical methods to estimate the impact of microstructure factors on corrosion properties. This study investigated how several microstructure factors affect corrosion rate in NaCl solution by using different evaluation models such as random forest algorism and multiple regression analysis and so on. Furthermore, the accuracy of the proposed model can be improved using additional data and applied to other alloys by changing the dataset.

*Keywords: Magnesium, Corrosion, microstructure, Machine learnings*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 9

November 22

16:00-18:00

# Technical **Oral Session _ Session 9**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 9-1 (A9-1)** — **16:00 – 18:00, Nov. 22**

**Chair** : Toshihiro Tsuchiyama (Kyushu University) — Halla Hall A, 3F

16:00-16:20 **I-A0752** **[Invited] Optimisation of Infill Structures in 3D Printed 316L Stainless Steels**
Zakaria Quadir (Curtin University, Australia)

16:20-16:40 **I-A0240** **[Invited] Hybrid additive manufacturing of 316L stainless steel**
Wen Hao Kan (The University of Sydney, Australia)

16:40-17:00 **I-A0403** **[Invited] Extraction of Process–Structure–Property Linkage Using Deep Learning Methods**
Junya Inoue (The University of Tokyo, Japan)

17:00-17:15 **O-A0016** **Sintering Pollutant Reduction Technology Based on Oxygen Redistribution**
Wen Pan (Beijing Key Laboratory of Green Recyclable Process for Iron & Steel Production Technology, China)

17:15-17:30 **O-A0761** **Reoxidation behavior of Al-killed ferritic stainless steel melts: Influence of tundish flux and Ti content**
Yeongjin Jun (Hanyang University, Korea)

17:30-17:45 **O-A0041** **Research on Corrosion Behavior of Weathering Bridge Steel in Simulated Typical Industrial Atmospheric Environment of Chemical Plant**
Sha Kaizhi (State Key Laboratory of Metal Material for Marine Equipment and Application, China)

17:45-18:00 **O-A0835** **Advancing mechanism of oxide/matrix interface for the internal oxidation of austenitic stainless steel in liquid lead-bismuth eutectic**
Chengxu Lu (Institute of Metal Research, Chinese Academy of Sciences, China)

# Optimisation of Infill Structures in 3D Printed 316L Stainless Steels

**Md Zakaria Quadir**[1], Ricardo Santamaria[2]

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## Abstract

This research presents the optimisation of infill design by additive manufacturing (AM) of 316L(SS316L) stainless steels by a sinter-based material extrusion technology. The goal is to achieve an overall weight reduction by exploiting the flexibilities offered by 3D printing in creating open and closed lattice cells. There is extensive research on the subject matter with polymeric materials, but only a limited study has been conducted with metallic materials. This study included two mechanical testing methods, the tensile and 3-point bend tests. The test samples were also examined with microscopy imaging and electron diffraction-based investigations to understand the distribution of applied stresses across the elements of the lattice structures. The obtained results were referenced against the fully solid specimens produced via 3D printing and conventionally manufactured wrought materials from commercial sources. The results show that the overall tensile properties vary with the relative density of the specimens. The study also reveals that under uniaxial stress conditions of the tensile testing, the load was primarily carried by the outer skin of the test specimen. The internal infill structures show the initiations of failure toward fractures. In comparison, the internal lattice structures play a significant role in the load-bearing in the multi-axial applied stresses of the 3-point bend test. These findings are obtained from the macro- and micro-scale microscopy investigations.

*Keywords: 3D Printing, Infill structures, EBSD, Mechanical Testing, Lightweight Structures*

# Hybrid additive manufacturing of 316L stainless steel

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## Abstract

One of the benefits of directed energy deposition, which is an additive manufacturing technique, is that it can be used simultaneously with other conventional manufacturing methods to manufacture parts. This approach is often referred to as hybrid manufacturing. In this study, a rolling apparatus was developed for use in a directed laser deposition system such that each layer of material can be rolled as it is being deposited. When applied to 316L stainless steel, hardness was increased by ~23% and yield strength by ~31%. These improvements were due to mechanical twinning, refinement of the cellular structure caused by solute micro-segregation, increased dislocation density, grain size reduction, and a randomization of the crystallographic orientation of the grains. Deformation-induced martensitic transformation was not observed. Furthermore, ductility was not compromised due to the reduction in porosity (from ~0.3% to ~0.02% with and without rolling, respectively). An additional benefit of the rolling process is that it can also help relieve residual stresses, as studies on post-weld rolling have shown. While the excellent corrosion resistance of the alloy was retained, the re-passivation, corrosion and pitting potentials were marginally affected by porosity closure and the stress-relieving effects induced by rolling. Therefore, this hybrid approach allows for the manufacturing of corrosion-resistant and ductile 316L parts that are stronger, harder, and denser without the need for additional post-process hot isostatic pressing or thermomechanical treatment steps.

*Keywords: Additive manufacturing, stainless steel, rolling, microstructure, corrosion*

# EXTRACTION OF PROCESS–STRUCTURE–PROPERTY LINKAGE USING DEEP LEARNING METHODS

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**Abstract**

The establishment of the process–structure–property linkage is essential for designing new materials with desired properties. Based on the concept, the discovery of new materials has been accelerated in the field of functional and bio-materials by combining quantum and molecular modeling tools with efficient machine learning methods. However, in the case of structural materials, even though the development of Integrated Computational Materials Engineering (ICME), it is still difficult to efficiently design new materials because of the uncertainties within models and experimental data. In this paper, our recent development of a general methodology for extracting the linkage between hierarchical microstructure and process conditions as well as properties will be reviewed. In the proposed method, the uncertainties will be captured in the form of probability density functions using deep learning methods. The framework is composed of two different functional components: one is for extracting geometrical features of material microstructures necessary to decompose each different microstructure, and the other is for clarifying spatial orders among the extracted characteristic components. The method was applied for generating virtual steel microstructures obtained after a certain continuous cooling process and those for desired mechanical properties. The obtained results show that the proposed methodology not only generates realistic microstructural images comparable to real experimental images but also clarifies a part of microstructures critically affecting the target property.

*Keywords: PSPP linkage, uncertainty, deep generative models, virtual microstructure, hotspot*

# Sintering Pollutant Reduction Technology Based on Oxygen Redistribution

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## Abstract

In this paper, the thermal characteristics of sintering flue gas are systematically studied, and the distribution law of flue gas flow, temperature, oxygen content, and NOx and other pollutants in the sintering process is obtained, and a mathematical model of sintered segmented oxygen excess coefficient is established.The model clarifies the oxygen demand for fuel combustion at different stages, and finds that in the longitudinal direction of the sintering machine, the oxygen demand for fuel combustion shows a trend of high and low before and after, especially in the middle and back stages of sintering, the demand for oxygen is greatly reduced.The measured results of a 550m$^2$ sintering machine show that after the 16# bellows, the flue gas with 15% concentration oxygen content can meet the fuel combustion in the material layer. Based on this theory, a cross-cycle process of sintering flue gas was developed, which reduced solid fuel consumption by more than 2kg/t and reduced the total amount of sintered pollutant emissions by more than 30%.

*Keywords: Sintering, Flue Gas Circulation, Oxygen, Excess Coefficient, Pollutants*

# Reoxidation behavior of Al-killed ferritic stainless steel melts: Influence of tundish flux and Ti content

**Yeong Jin Jun [1]**, Sung Jin Park[2], Soo Chang Kang[2], Joo Hyun Park[1,*]

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## Abstract

According to the global carbon neutral policy, the hydrogen energy market is growing and the interests in hydrogen fuel cells is growing too. For the fuel cell separator, the Ti-containing ferritic stainless steels are used due to their high corrosion resistance, electrical conductivity, and durability. The refining of Ti-added ferrite stainless steel and the relevant cleanliness have been improved *via* vacuum-oxygen decarburization (VOD) and ladle treatment (LT) processes. However, the reoxidation phenomena occur during melt transfer from ladle to continuous casting tundish, resulting in a loss of titanium yield in conjunction with a formation of reoxidative inclusions. Hence, the present work aims to investigate the combinational effect of different tundish fluxes on the reoxidation behavior of Al-killed stainless steel melts containing Ti. Rice husk ash (RHA) and MgO (M) cover powders, and CaO-$Al_2O_3$ (CA) based flux were used for the experiments with various combinations. A decrease of total oxygen content was largest in M+CA combination experiments. Also, the main type of inclusion was changed according to the combination of fluxes: main type of inclusions in M+CA system was $Al_2O_3$ and liquid $Ti_2O_3$-$Cr_2O_3$-$Al_2O_3$ system inclusions. However, $Al_2O_3$ and liquid $Ti_2O_3$-$Cr_2O_3$-$Al_2O_3$ -$SiO_2$ system inclusions were observed in RHA-added combinations.

Alternatively, when the Ti/Al ratio was relatively low, the inclusions are able to produce alumina clusters. Hence, the removal efficiency of inclusions were highest at low Ti/Al conditions. Consequently, the cleanliness of molten ferritic stainless steel containing different Ti contents was improved under the CA+M combination as well as low Ti/Al ratio.

*Keywords: Fuel cell separator, Ferritic stainless steel, Tundish, Reoxidation, Inclusion*

# Research on Corrosion Behavior of Weathering Bridge Steel in Simulated Typical Industrial Atmospheric Environment of Chemical Plant

**Kaizhi Sha**[1], Yiqing Chen[2], Bin Zhong[3], Peng Gao[4], Lin Li[5], Fangfang Ai[6], Xiandong Su[7],Hongyu San[8], Shengjie Zhang[9]

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## Abstract

In the chemical plant industrial atmospheric environment, periodic infiltration and long-term soaking tests were used to simulate the actual service environment. The corrosion behavior of Q420 and Q690 weathering bridge steel in the simulated chemical plant industrial atmospheric environment was studied by using the weight loss method, corrosion morphology observation and electrochemical analysis. The results showed that the surface: nitrate ion has certain corrosion inhibition effect on weathering bridge steel. In the environment of high chloride ion concentration, the corrosion inhibition effect of nitrate ion is better.

*Keywords: Weather resistant bridge steel, Weather resistant bridge steel, Corrosion, Nitrate ion, Corrosion inhibition.*

# Advancing mechanism of oxide/matrix interface for the internal oxidation of austenitic stainless steel in liquid lead-bismuth eutectic

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Currently austenitic stainless steels are considered as promising candidate materials for the fuel cladding tubes in lead-cooled fast reactors, owing to their exceptional high-temperature mechanical properties, processability, and resistance to lead-bismuth eutectic (LBE) corrosion embrittlement. According to the existing literature, investigations are made on the LBE corrosion mechanism of austenitic stainless steels but still insufficient, especially for the advancing process of the oxidation frontier, or the oxide layer/matrix (O/M) interface. In this study, the internal oxidation behavior of 15-15Ti austenitic stainless steel in the 550°C (6000 h Max) oxygen-saturated static LBE was systematically investigated, in which the chemical composition, phase structure, interfacial characteristics and morphology evolution of the oxide film were studied in detail by multiple characterization methods. Results indicate that 15-15Ti forms a multilayered oxide structure which generally including an outer layer of $PbFe_4O_7$ + $Fe_3O_4$, and a non-uniform $FeCr_2O_4$ spinel structure as the inner layer. The thickness of each oxide layer was measured and the kinetic growth laws of them were analyzed. Notably, distinctive structures were observed within the inner oxide layer, such as the Cr-Si-rich complex oxides at previous grain boundaries, the island-like areas enriched with Ni, and the tree-ring-like traces following the oxidation frontier. These morphology characteristics provide more details and clues to elucidate the internal oxidation mechanism of this alloy.

The O/M interface of 15-15Ti are often found protruding like a spike towards the matrix when it goes across the grain boundary of alloy. Usually grain boundaries are considered as the short-circuit diffusion channels for oxygen, but the pathway of oxygen diffusion and the oxidation process of grain boundary are scarcely described in the existing literature. According to the FIB-STEM characterization, it is discovered that the intergranular oxide possesses a sandwich structure as $Cr_2O_3$/$SiO_2$ (amorphous)/$Cr_2O_3$. Specifically, $Cr_2O_3$ grows on the surface of amorphous $SiO_2$ and tends to encase it. With the in-diffusion of oxygen, the complex oxides form at the forefront of O/M interface and proceed on the grain boundary. Some special blocky areas can be occasionally found on the grain boundary. Moreover, it is interesting that when confronts these blocky areas, the oxides deviate from their previous growing direction, pass around the blocky area, and then return to the grain boundary retrieving their previous growing pattern. EDS investigations show that these blocky areas are highly enriched in Ni. Previous researches once reported the existence of island-like Ni-rich areas which regarded as the remnants of matrix oxidation. However, by using a layer-by-layer mechanical polishing technique, we found that these blocky Ni-rich areas origin from the matrix not yet oxidized. Furthermore, EBSD studies indicate that these intergranular Ni-rich areas shear the same orientation with the adjacent grain and grow into the grain on the other side. In other words, the formation of Ni-rich areas can induce grain boundary migration and suppress the advance of O/M interface, thereby enhancing the anti-corrosion property of alloy in LBE. In addition, microstructure of the O/M interface within grains were characterized as "Fe-Cr spinel / $Cr_2O_3$ / $SiO_2$ (armorphous) / matrix". Considering the tree-ring-like traces behind the O/M interface, one can infer that the intracrystalline oxidation interface advances in an "obstruction-breakthrough-obstruction" mode rather than in an even pace.

This work discusses the formation mechanisms of special oxide structures, establishes a new internal oxidation mode, and introduces the effects of silicon and aluminum on the anti-corrosion performance of 15-15Ti.

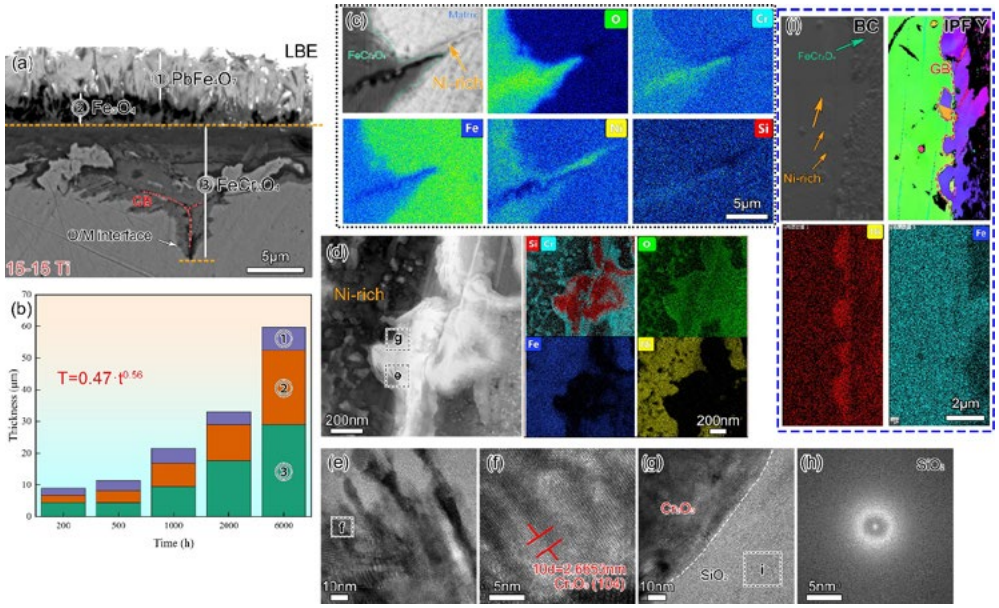



**Fig.** Cross-section morphology (a) and oxide films thickening rate (b) of 15-15Ti, O/M interface oxide film composition (c-d) and structure (e-h) analysis, EBSD analysis of Ni-rich areas (i).

**Keyword**. Lead-cooled fast reactor, Austenitic stainless steel, LBE corrosion, Oxidation

# Technical **Oral Session _ Session 9**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 9-2 (A9-2)** **16:00 – 17:45, Nov. 22**

**Chair :** Yoshikazu Todaka (Toyohashi University of Technology) 303B, 3F

16:00-16:15 **O-A0022** **The effect of Co and Cu on grain growth kinetics in ferritic/martensitic heat-resistant steels**
Bong Cheon Park (Korea Institute of Material Science, Korea)

16:15-16:30 **O-A0857** **Transition of deformation mode from dislocation slip to martensite transformation with grain refinement in an austenitic stainless steel**
Dapeng Yang (Northeastern University, China)

16:30-16:45 **O-A0301** **Relation between misorientation of prior austenite grain boundary (PAGB) and hydrogen-induced crack propagation path**
Ji Hoon Kim (Tohoku University, Japan)

16:45-17:00 **O-A0149** **Exploring the Impact of Grain Boundary Character Distribution on the Hall-Petch Relationship in Austenitic Stainless Steel, SUS316L**
Misato Nakajima (Kumamoto University, Japan)

17:00-17:15 **O-A0034** **The influence of pre-plating on the LME phenomenon during spot-welding of DH780 advance high strength steel**
Xue Bai (Shougang Group Co., Ltd, China)

17:15-17:30 **O-A0942** **Impact of Post Weld Heat Treatment on Stress Relaxation Cracking in 347H Weldments**
Zhenzhen Yu (Colorado School Of Mines, USA)

17:30-17:45 **O-A1121** **Direct 3D Atomic-Scale Insights into Weak and Strong Hydrogen Trapping Sites in High-strength Cold-drawn Steels**
Chao Huang (The University of Sydney, Australia)

# The effect of Co and Cu on grain growth kinetics in ferritic/martensitic heat-resistant steels

**Bong cheon Park**[1], Jae Hoon Jang[2], Tae-Ho lee[3], Tae-Ho lee[3], Sung-Dae Kim[4]

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## Abstract

Ferritic/martensitic heat-resistant steels containing 9-12 wt% Cr are widely used in thermal power plants as materials for rotors and blades due to their excellent thermal stability, conductivity and low thermal expansion coefficient. However, high temperature exposure under process condition can lead to austenite grain growth, which in turn can affect thermal properties and reduce the creep life of the materials. Therefore, controlling the grain size is crucial to improve the creep life of these materials.

This study investigated the effect of Co and Cu on austenite grain growth kinetics in ferritic/martensitic heat-resistant steels. Three alloys with different Co and Cu contents were produced based on an alloy composition of 10.2Cr-Mo-W-V-Co-C-Nb, which is designed for thermal power plants. Each alloys was heat-treated from 1050℃ to 1200℃ for up to 4 hours, and the prior austenite grain size was measured from optical microscopic images. The results showed that decreasing Co content and increasing Cu content inhibited prior austenite grain growth. Scanning electron microscopy and transmission electron microscopy analyses were also conducted to examine the microstructure of the alloys. Empirical equations were derived based on the measured austenite grain size, and grain growth simulations were conducted using MatCalc software to quantify the effect of Co and Cu on austenite grain growth. The results showed that Co and Cu had a significant effect on grain growth kinetics, and their influence could be predicted by the simulation.

In conclusion, this study provides valuable insights into the effect of Co and Cu on grain growth kinetics in ferritic/martensitic heat-resistant steels. The results can be used to optimize the alloy composition and process condition to improve the creep life of ferritic/martensitic steels.

*Keywords: F/M Heat-resistant steels, Prior austenite grain growth kinetics, effect of Co and Cu, Austenite growth modelling.*

# Transition of deformation mode from dislocation slip to martensite transformation with grain refinement in an austenitic stainless steel

**Dapeng Yang[1],** Tao Wang[1], Zhitong Miao[1], Guodong Wang[1], Hongliang Yi[1]

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## Abstract

An austenitic stainless steel was employed to clarify the intrinsic effect of grain size on the mechanical stability of austenite in transformation-induced plasticity (TRIP) steels. Contrary to the general impression in TRIP-assisted steels with multi-phase microstructure, the austenite mechanical stability decreases as the grain size decreases in the single-phase austenitic steel. The unexpected phenomenon was explained in the essence of austenite mechanical stability by theoretical calculation and experimental verification: dislocation slip and martensite transformation are two competing deformation mechanism during plastic deformation of austenite, the stress for martensite transformation will be lower than that for dislocation slip when the grain size is smaller than a critical value. Therefore, the yielding mechanism of austenite will transit from dislocation slip to martensite transformation with the refinement of austenite grains.

*Keywords:* Grain size; Austenite mechanical stability; Deformation mechanism; Martensite transformation; Dislocation slip

| O-A0301 |

# Relation between misorientation of prior austenite grain boundary (PAGB) and hydrogen-induced crack propagation path

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## Abstract

This study investigated the hydrogen-induced crack propagation path in SCM435 tempered martensitic steel. The hydrogen-induced crack was introduced by U-bending, and subsequent hydrogen charging. The result shows that the major crack propagation path was prior austenite grain boundary (PAGB). The PAGB crack propagation path was analyzed in terms of misorientation of martensite ($\theta_{\alpha'}$) and prior austenite ($\theta_{\gamma}$). The cracks could hardly propagate along PAGB with low $\theta_{\alpha'}$ and $\theta_{\gamma}$. Specifically, it was found out that the length fraction of low $\theta_{\alpha'}$ (<15°) at PAGB ($f_{low\ \theta\alpha'}$) is an important factor in suppressing PAGB cracking. The statistical result revealed that the $f_{low\ \theta\alpha'}$ greater than 0.4 is necessary to suppress PAGB cracking. The $f_{low\ \theta\alpha'}$ of low $\theta_{\gamma}$ (<10°) PAGBs was usually higher than 0.4, which is the reason why PAGB cracking was not observed in low $\theta_{\gamma}$ (<10°) PAGBs. However, the $f_{low\ \theta\alpha'}$ of intermediate $\theta_{\gamma}$ ($10°<\theta_{\gamma}<50°$) PAGBs was usually lower than 0.4 due to inter-variant misorientation angles among 24 K-S martensite variants across PAGB. For high $\theta_{\gamma}$ (>50°) PAGB, although $f_{low\ \theta\alpha'}$ of most of the PAGBs was less than 0.4, PAGBs with $f_{low\ \theta\alpha'}$ over 0.4 were often observed. Observation on initial martensite nucleation at PAGB by applying interrupted quenching treatment revealed that the high-angle PAGB ($\theta_{\gamma}>50°$) tends to have high $f_{low\ \theta\alpha'}$ when it was the initial martensite nucleation site.

*Keywords: Hydrogen embrittlement, Hydrogen delayed fracture, Martensitic steel, Prior austenite grain boundary (PAGB)*

# Exploring the Impact of Grain Boundary Character Distribution on the Hall-Petch Relationship in Austenitic Stainless Steel, SUS316L

**Misato Nakajima[1],** Takateru Yamamuro[2], Sadahiro Tsurekawa[3]

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## Abstract

Grain boundaries (GBs) significantly impact material mechanical properties, as described by the Hall-Petch relation. According to the dislocation pile-up model, the Hall-Petch coefficient $k_y$ includes the critical stress $\tau_c$ required to propagate plastic deformation across the grain boundary to the adjacent grains. Previous fundamental studies have confirmed that the properties of GBs can vary in multiple ways depending on their character and structure. It is anticipated that the critical stress $\tau_c$ is influenced by the character and structure of GBs. Recent studies utilizing nanoindentation techniques have indicated that the critical stress necessary for propagating plastic deformation depends not only on the misorientation but also on the orientation of the GB plane. Consequently, the distribution of grain boundary character distribution (GBCD) is expected to impact the Hall-Petch coefficient $k_y$. A comprehensive understanding of the physical significance of the Hall-Petch coefficient would enable further enhancements of material strength via control of GBCD as well as grain size.

To investigate the influence of GBCD on the Hall-Petch relation, tensile tests were conducted on several samples of austenitic stainless steel, SUS316L with similar fraction of Coincident Site Lattice (CSL) boundaries and the same grain size. These samples were prepared through thermomechanical treatment.

Distinct groups of specimens were successfully obtained, each having different fractions of CSL boundaries. Our findings demonstrate that the data from each group conform well to the Hall-Petch relationship. Importantly, our results reveal a dependency of the Hall-Petch slope, $k_y$, on the fraction of CSL boundaries.

(244 words)

*Keywords: Grain Boundary Character Distribution, Grain Boundary Engineering, Hall-Petch relation, tensile test, stainless steel*

# The influence of pre-plating on the LME phenomenon during spot-welding of DH780 advance high strength steel

**Xue Bai**[1], Yun Han[2], Guangrui Jiang[3], Huasai Liu[4], Yongwei Wang[5]
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## Abstract

The advanced high strength steel has been used in the automobile plate for the light-weight purpose. The galvanized steel plate is developed to protect the car from corrosion. During the resistance spot-welding, the liquid metal embrittlement (LME) phenomenon occurs because of the lower melting temperature of zinc or zinc intermetallic compounds, then the melted Zn would get penetrated into grain boundaries which would cause the embrittlement. The LME index has been employed to evaluate the mechanical properties. The pre-plating technology has been proved could improve the LME resistance property of the galvanized steel. The microstructure analysis shows that the LME micro-cracks could be reduced. It could also be concluded from the gleeble test results that the crack time could be postponed after the pre-plating technology.

*Keywords: Advanced high strength steel, Resistance spot-welding, Liquid metal embrittlement (LME), Pre-plating*

# Impact of Post Weld Heat Treatment on Stress Relaxation Cracking in 347H Weldments

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**Abstract**: Stress relaxation cracking (SRC) has been reported as one of the main mechanisms contributing to failures in austenitic steels in multiple countries in heat-affected zone (HAZ) and weld metal, particularly in HAZ without post weld heat treatment (PWHT). In this study, a fundamental understanding of the failure conditions in 347H stainless steel welds was achieved by combining finite element modeling, residual stress mapping, thermodynamic calculations, thermomechanical experiments, and metallurgical characterizations. Furthermore, stress evolution profile as a function of temperature, time, and insulation conditions during PWHT was investigated through finite element (FE) simulation, which was validated by neutron diffraction measurement of residual stress distributions before and after PWHT. Proper PWHT parameters were thereafter down selected for the purpose of stress relieving while avoiding SRC to occur during heat treatment. The impact of PWHT on susceptibility of 347H stainless steel weldments to SRC under service condition is further evaluated through thermomechanical testing and metallurgical characterization.

**Keywords:** Stress relaxation cracking, 347H stainless steel, post weld heat treatment, residual stress

# Direct 3D Atomic-Scale Insights into Strong Hydrogen Trapping Sites in High-strength Cold-drawn Steels

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## Abstract

Mobile hydrogen atoms within high-strength steels can lead to hydrogen embrittlement. One effective approach is to incorporate hydrogen traps into material microstructure. It is thus crucial to understand which microstructures are more adept at trapping hydrogen to create materials that are resistant to embrittlement. In the case of cold-drawn pearlitic steels, the microstructures are intricate and pose challenges when using traditional methods, such as hydrogen thermal desorption analysis, to correlate hydrogen trapping with these complex structures. As such, we employed advanced microscopy techniques like transmission electron microscopy and atom probe tomography, in combination with mechanical testing, to investigate the hydrogen trapping and hydrogen embrittlement in pearlitic steels subjected to various levels of cold drawing. Our research developed a new method to evolute the ability of H trapping and revealed that sessile dislocations blocked by cementite-ferrite interfaces, and strained interface with interfacial dislocations are as strong H trapping sites and play a pivotal role in trapping hydrogen, which virtually locks moving hydrogen atoms, reducing the risk of hydrogen embrittlement. This finding can be used to facilitate the material design that can enhance the overall hydrogen embrittlement resistance.

*Key words: Iron and Steel, Characterization, Environmental Effects*

# Technical **Oral Session _ Session 9**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 9 (B9)** — **16:00 -17:40, Nov. 22**

**Chair :** Antonella Sola (CSIRO Manufacturing) — 301, 3F

16:00-16:20 **I-B0480** **[Invited] Processing-related challenges in fused filament fabrication of composite materials**
Antonella Sola (Commonwealth Scientific and Industrial Research Organisation, Australia)

16:20-16:40 **I-B0568** **[Invited] Increasing electrical anisotropy and current waveform response of soft, flexible 3D printed sensors through material formulation**
Dejana Pejak Simunec (CSIRO Manufacturing, Australia)

16:40-16:55 **O-B0467** **A Fundamental Study on Laser-patterned Surface of Metals for Improving Metal-composite Bonding Force**
Junyeong Jeong (Hyundai Motor Company, Korea)

16:55-17:10 **O-B0087** **Research and development of coating thickness uniformity control technology for hot dip galvanizing coating plate**
Jing Fei (Anshan Iron And Steel Co., ltd. China)

17:10-17:25 **O-B0450** **Investigation of In-situ Cutting Temperature in Machining Bone Substitute Material with Steel and Ceramic Tools**
Saiful Anwar Che Ghani (Universiti Malaysia Pahang, Malaysia)

17:25-17:40 **O-B1108** **Achieving simultaneous high strength and ductility via accumulative skin pass rolling**
Rui Wang (University of Wollongong, Australia)

# Processing-related challenges in fused filament fabrication of composite materials

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## Abstract

Fused filament fabrication, FFF (a.k.a. fused deposition modeling, FDM) is currently the most widespread additive manufacturing (AM) technique to produce plastic parts. In principle, the process is straightforward, since a thermoplastic polymer-based filament is fed into a 3D printer, heated, melted, and extruded layer-by-layer to complete the desired component. However, the limited functionality of thermoplastic materials that are routinely processed in FFF is hampering the industrial uptake of this technology. Composite materials are thus needed to provide FFF parts with new functionality and customisable features that can be tailored to match the assigned service requirements. While the addition of functional fillers is key to opening up new opportunities for FFF of innovative materials, processing-related challenges arise due to the altered printability of the polymer matrix. The establishment of a consistent manufacturing procedure that encompasses all the steps from composite filament preparation to printing to finishing becomes crucial to satisfying the requirements of high-performance areas of aerospace, defence, and biotech.

This contribution discusses the state of the art in incorporating functional fillers into FFF, and highlights strategic case-studies being developed at the 4F, CSIRO's research hub for composite and advanced materials for FFF and material extrusion AM.

*Keywords: composite material; thermoplastic; fused filament fabrication; fused deposition modeling; additive manufacturing.*

# Increasing electrical anisotropy and current waveform response of soft, flexible 3D printed sensors through material formulation

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## Abstract

Rising interest from the smart electronics industry in 3D printable sensors has been driven by the limitless choice of geometries and rapid prototyping options enabled by the printing process. Moreover, bespoke feedstock materials can be imbued with a variety of specific properties desired in the final product. Specifically, piezoelectric and conductive fillers can be incorporated within a polymer matrix to obtain flexible sensor. However, piezoelectricity must be activated by poling, which consists in applying a potentially dangerous high voltage electrical field. To reduce this risk, we present a polymer-based material that can be printed into soft and flexible sensors that are conductive and contain piezoelectric elements. We investigate several non-poling techniques to understand their effect on the electrical characteristics of the 3D printed parts. It was found that a combination of these techniques leads to significantly higher sensor responses with respect to the untreated parts. In addition, electrical anisotropy was governed through the orientation of 'sea-island' structures induced by the composite formulation and the shear forces generated by the printing process. The results discussed within this study highlight the importance of tuning the composite formulation and applying appropriate non-poling treatments before any piezoelectric sensor is activated under an electric field.

*Keywords: soft robotics, 3d printing, polymer, composites, sensors*

# A Fundamental Study on Laser-patterned Surface of Metals for Improving Metal-composite Bonding Force

**Junyeong Jeong[1],** Chang-Yeol Yoo[1], Youn-Il Jung[1], Changkyoo Park[2], Sanghyun Hong[3], Jongyoon Kim[4]

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## Abstract

An automotive industry has been focusing on importance of light-weighting to reduce emissions and increase fuel efficiency and driving range. To achieve the weight reduction goal, an application of reinforced plastic with glass or carbon fiber to a car body has been actively considered due to its lightweight compared to structural metals such as steel and aluminium alloy. However, high materials price and low productivity of the fiber-reinforced plastic (FRP) composite limit its applications in the car body. Therefore, hybrid technologies that can locally apply FRP composite to existing steel or aluminium car body parts have been developing with various methods. To apply metal-composite hybrid structures to the car body, the metal and composite must be strongly bonded, but due to the difference of material properties such as melting point and thermal expansion ratio, it is difficult to join them using conventional welding methods. To overcome the problem, we studied a joining method to reinforce the boning force between metal-FRP composite applying two joining technologies: Injection molding and automated fiber placement (AFP). In this research, 1470 MPa-grade steels and Al-Mg-Si aluminium alloys were used and PA6/GF50 and RENY/CF50 tape were used in joining methods of injection molding and AFP, respectively. We carried out lap-shear tensile test to estimate the bonding force and bending test to analyse the stiffness of the metal-composite bonded specimens according to the type of laser-textured patterns including pattern depth, gap, and directions.

*Keywords: metal-composite hybrid, laser texturing, injection moldling, automated fiber placement*

# Research and development of coating thickness uniformity control technology for hot dip galvanizing coating plate

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**Abstract**

In this paper, based on the background of cold rolling hot dip galvanizing production line, the main factors affecting the control accuracy of coating thickness uniformity of hot dip galvanizing coating plate were analyzed through numerical simulation of gas knife flow field during air knife injection process.The prediction model of coating thickness uniformity of hot dip galvanizing coating plate has been established，as well as a time-varying model-free controller and a robust model-free controller of the air cutter. The precise control effect of the coating thickness uniformity for hot dip galvanized coating plate was achieved . The results of the production data show that the thickness deviation of the coating was reduced through the application of the coating thickness uniformity control technology, and acquired the better control effect . The application of coating thickness uniformity control technology not only meets the demand of improving product surface quality，but also provides an important significance on cost saving and reducing the zinc raw material consumption .

*Keywords:hot dip galvanizing;coating thickness uniformity;time-varying model-free controller ;robust model-free controller*

# Investigation of In-situ Cutting Temperature in Machining Bone Substitute Material with Steel and Ceramic Tools

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## Abstract

In orthopaedic surgery, excessive heat generation during the machining process can cause permanent cell damage in bone tissue, known as osteonecrosis. To minimize heat generation and cutting temperature, various parameters have been studied, such as tool design, tool material, optimal cutting parameters, and cooling delivery. In this study, we assess the real-time temperature distribution in a surgical-grade bone substitute workpiece (40 pcf density) during machining with innovative zirconium oxide ceramic and stainless steel 316L cutting inserts. The study was conducted in two steps: first, zirconium oxide ceramic powder was sintered in Hyderabad, India, to produce high-integrity cutting inserts; then, cutting trials were performed on a CNC machine tool in Pekan, Malaysia, with different cutting conditions. Eight k-type thermocouples were embedded inside the workpiece to acquire the online temperature distribution during face milling processes with SS316L and Zr-based tools at varied cutting parameters, i.e., cutting speed, feed rate, and axial depth of cut, which were set at (900 and 1000) m/min, (0.03 and 0.05) mm/tooth, and 1.3 mm, respectively. The maximum cutting temperature recorded for each cut is presented in box plots, indicating that both tools cut at a temperature below 45 °C. At high speed, both cutting tools performed similarly well, but at low speed, the performance of the SS316 tool dropped, and the cutting temperature exceeded 40 °C. This may be due to longer friction duration between the tool and the uncut surface, resulting in higher heat generation and conduction to the workpiece. The cutting temperature increased with increasing feed, but overall, the Zr-based tool performed better than the SS316L tool. Our findings suggest that ceramic-based cutting inserts are a good alternative to steel-based cutting inserts in orthopaedic surgery, as they not only improve productivity with higher cutting speed and feed rate but also avoid thermomechanical damage to bone tissue.

*Keywords: In-situ cutting temperature, osteonecrosis, ceramic insert, real time data acquisition, zirconium oxide, bone substitute.*

# Achieving simultaneous high strength and ductility via accumulative skin pass rolling

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## Abstract

In the pursuit of high strength, severe plastic deformation is often employed at the expense of ductility. The simultaneous enhancement of both strength and ductility to overcome this trade-off in metallic materials has garnered significant attention. This study introduced a novel approach, named accumulative skin pass rolling, applied to an annealed pure copper to improve its mechanical properties. Through accumulative skin pass rolling, involving hundred passes and total 10% reduction, a favourable combination of high strength and acceptable ductility is achieved. The microstructural evolution of the rolled samples is examined using Electron Backscatter Diffraction (EBSD) analysis, comparing it with the initial annealed state. Interestingly, the average grain size exhibits minimal deviation between the initially annealed copper and the accumulative skin pass rolled samples. Detailed observations reveal a heterogeneous distribution of low-angle grain boundaries spanning the material's thickness. These boundaries, coupled with misorientation analysis, shed light on the underlying mechanisms contributing to enhanced strength. Numerical simulations corroborate these findings, depicting a heterogeneous strain distribution akin to the microstructural profile. The synergy between microstructural characterization and numerical simulations indicates that multiple surface rolling induces strain hardening predominantly at the sample's surface, while the interior experiences either elastic deformation or partial plastic deformation. This deliberate heterogeneity in deformation results in a metal sheet endowed with both high strength and ductility, presenting a promising advancement in materials engineering.

*Keywords: Advanced Processing; rolling; heterogeneous deformation; crystal plasticity.*

# Technical **Oral Session _ Session 9**

## **Symposium C :** Structural Materials for High Temperature

**Structural Materials for High Temperature 9 (C9)** **16:00 - 18:05, Nov. 22**

**Chair :** Bin Lee (Kyung Hee University) 201A, 2F

16:00-16:30 **K-C** **[Keynote]**
Guoqing ZHANG (AECC Beijing Institute of Aeronautical Materials, China)

16:30-16:50 **I-C0536** **[Invited] Effect of Impurities on Creep Strength and Microstructure in Welded Joints of High-Cr Ferritic Heat Resistant Steel**
Masatoshi Mitsuhara (Kyushu University, Japan)

16:50-17:05 **O-C0123** **Radiation-Induced Effects on Microstructure and IASCC Susceptibility of Austenitic 316 Stainless Steel**
Yun Soo Lim (Korea Atomic Energy Research Institute, Korea)

17:05-17:20 **O-C0555** **Ex-situ observation of microstructure evolution during aging at 1013 K in 9Cr ferritic steel weld metal**
Katsuhiro Sato (IHI Corporation, Japan)

17:20-17:35 **O-C0631** **Microstructure Characteristics and Mechanical performance of Transformable 9Cr ODS Steels with Different Types of Minor Alloying Additions**
Xiaosheng Zhou (North University of China, China)

17:35-17:50 **O-C0454** **Unveiling the Re effect on microstructural stability, high-temperature strength of high-Cr CoNi-based superalloy**
Xiaorui Zhang (University of Science and Technology Beijing, China)

17:50-18:05 **O-C1134** **Revealing the Microstructural Evolution and Strengthening Mechanisms of Additively Manufactured Ni-based Hastelloy X Superalloy**
Seung-Chang Han (Incheon National University, Korea)

# Effect of Impurities on Creep Strength and Microstructure in Welded Joints of High-Cr Ferritic Heat Resistant Steel

**Masatoshi Mitsuhara**[1], Katsuhiro Sato[2], Kyohei Nomura[2], Yoshiki Shioda[3], Kota Sawada[4], Kazuhiro Kimura[4], Hideharu Nakashima[1]

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## Abstract

High-chromium (Cr) ferritic heat-resistant steels, such as ASME Gr.91 steel are used for steam pipes in thermal power plants. ASME (2019) divided SA335 P91 into two standards, Type-I and Type-II. Type-II restricted impurities such as As, Sb and Sn, and established higher allowable stress compared to Type I. However, few research reported impurity effects on the creep strength and microstructures of the welded joint. In this study, the high-temperature strength of two welded joints with different impurity concentrations was investigated by creep tests under several conditions. The results showed that the specimens with higher impurity concentrations had lower strength. During welding, a heat affected zone (HAZ) is created, and the microstructure of the HAZ changes depending on the distance from the fusion line. We developed a method to clearly classify the microstructure of the HAZ based on crystallographic orientation information and hardness. The relationship between creep strength and microstructure of the HAZ was analysed in detail to investigate the effects of impurities on them. The steel had a lath martensitic microstructure. The fracture was caused by the recovery and recrystallization of the fine-grained part of the weld heat-affected zone (FGHAZ) under the influence of temperature and stress during creep deformation. The amount and distribution of carbides were responsible for this microstructural change in the FGHAZ. In the impurity-rich samples, carbides were less likely to re-solidify during the welding process, and therefore the number density of carbides precipitating on the grain boundaries during post-weld heat treatment was reduced. It suggests that the resistance against microstructural recovery during creep was reduced. The impurities thus degraded the creep strength of the welded joints.

*Keywords: High-Cr ferritic heat-resistant steels, Weld joint, Creep, Microstructure, Impurities*

# Radiation-Induced Effects on Microstructure and IASCC Susceptibility of Austenitic 316 Stainless Steel

**Yun Soo Lim[1],** Dong Jin, Kim[2], Sung Woo Kim[3], Seong Sik Hwang[4], Sung Hwan Cho[5]

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## Abstract

Irradiation-assisted stress corrosion cracking (IASCC) of austenitic 316 stainless steel (SS), commonly used in the internal components of a pressurized water reactor (PWR), is considered critical for safe long-term operation. The IASCC mechanism is not fully understood, though it appears to be closely related to microstructural changes caused by neutron irradiation. Proton irradiation is a well-known useful experimental technique to study neutron irradiation-induced phenomena. Proton irradiation can produce a microstructure and microchemistry very similar to those of neutron irradiation. The objectives of the present work are to investigate the microstructural features and cracking behaviour of proton-irradiated 316 SS to obtain clear insight into the role of irradiation defects in PWR primary water.

Point defects, Frank loops, and dislocations were found mainly in the area exposed to a low radiation dose; however, voids were dominant in areas exposed to a high radiation dose. Ni, Si, B and P were enriched, whereas Cr, Mn and Mo were depleted on the grain boundaries associated with radiation-induced segregation (RIS). From slow strain rate tests, it was demonstrated that the IASCC susceptibility of proton-irradiated 316 SS increased depending on the radiation dose. The promotion of the diffusion of alloying elements by irradiation defects, the severe depletion of Cr along the grain boundaries by RIS and surface oxidation, and the easy rupture of the protective surface oxidation layers by pile-up dislocations at a grain boundary, including degradation of the mechanical properties caused by irradiation hardening, appear significantly to increase the IASCC susceptibility of austenitic 316 SS.

Topic area: C (Structural Materials for High Temperature)

*Keywords: Austenitic 316 Stainless Steel, Proton Irradiation, Irradiation Defects, RIS, IASCC*

# Ex-situ observation of microstructure evolution during aging at 1013 K in 9Cr ferritic steel weld metal

**Katsuhiro Sato[1],** Akihiro Shin[2], Masatoshi Mitsuhara[3], Hideharu Nakashima[3]
Kyohei Nomura[1], Yohei Sakakibara[1], Keisuke Togrigata[1] and Yoshiki Shioda[4]

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## Abstract

9Cr-1Mo-V-Nb steel is commonly used in thermal power generation plants. Although initial microstructures of base metal and weld metal of the steel are mostly martensite structure, it has been reported that coarsened ferrite grains were occasionally observed in the weld joint after long-term use. Unfortunately, few studies have reported detailed examinations of such microstructures in the weld metal. This study was conducted to investigate ferrite growth behaviour using ex-situ observation method. Ex-situ observation means observation of a same field of view and aging heat treatment alternatively. Aging was conducted at 1013 K. Before the aging, microstructure of the as-welded metal was observed. The observation indicated that most part of initial microstructure was martensite. Also, small quantity of ferrite with irregular shape was observed near fusion line. Dislocation density inside the ferrite grain was relatively low. However, it has not been concluded whether the ferrite derived from δ-ferrite or microstructural changes of martensite by welding thermal cycles. Ex-situ observation revealed that the ferrite grain slightly grew and consumed surrounding martensite structure. Unexpectedly, grain growth rate of the ferrite was slow. After 500 h aging, however, a coarsened ferrite grain was suddenly appeared in which the original microstructure was martensite. It suggested that microstructural change from martensite to ferrite was occurred during the aging. Moreover, grain growth of such ferrite was significantly faster than that of the other ferrite existing in the as-welded metal. Difference in features between the two kinds of ferrite will be discussed on the day of presentation.

*Keywords: High Cr ferritic steel, EBSD, Ferrite, Grain growth*

概要
9Cr-1Mo-V-Nb 鋼は火力発電プラントに広く使用されている．9Cr-1Mo-V-Nb 鋼母材および溶接金属の初期組織は大部分がマルテンサイト組織であるが，長期使用された同鋼溶接部においてフェライトが観察される事象が報告されている．しかしながら溶接金属における組織変化を詳細に調査した例は多くは無い．そこで本研究では，9Cr-1Mo-V-Nb 鋼溶接金属におけるフェライトの粒成長挙動を ex-situ 観察により調査した．Ex-stiu 観察は同一視野の観察と時効を繰り返し行う実験である．時効する前に，溶接まま材の初期組織を観察した．溶接まま材の初期組織の大部分はマルテンサイト組織であったが，溶接線近傍にフェライトが観察された．フェライト内部の転位密度は定性的に低かった．このフェライトはδフェライトに相当するか，もしくは溶接熱影響により組織変化した組織である可能性が考えられるものの，どちらに由来するかを結論することはできていない．1013K で時効したところ，フェライトがわずかに粒成長し，周囲のマルテンサイト組織を蚕食する様子が観察された．予想に反して，フェライトの粒成長速度は遅かった．ところが 500h 時効後に，元々はマルテンサイト組織が存在していた領域に粗大なフェライト粒が観察された．これらの観察結果から，マルテンサイトからフェライトへの組織変化が時効中に生じたことが示唆される．また，時効中に生成したフェライトの粒成長速度は溶接まま材で観察されたフェライトのそれと比べて優位に速かった．発表当日は本研究で観察された二種のフェライトの特徴とその差異について議論する予定である．

# Microstructure Characteristics and Mechanical performance of Transformable 9Cr ODS Steels with Different Types of Minor Alloying Additions

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## Abstract

Oxide dispersion strengthened (ODS) steels have been considered as the preferential structural materials for nuclear reactors, owing to their superior radiation resistance, excellent creep resistance and high-temperature tensile strength. Aimed at increasing the maximum use temperature of ODS steels, various types of minor alloying elements were respectively added into the 9Cr ODS steels, including Al, Ti, Zr and Hf. These added minor alloying elements would affect the transformation behaviour and microstructure characteristics of ODS steels. Size distributions of Y-Al-O, Y-Ti-O, Y-Zr-O and Y-Hf-O were studied, as well as their orientation relationships with the matrix. Compared to Al addition, Ti or Zr addition indeed effectively retarded the formation of coarse $M_{23}C_6$ in transformable ferrite, and the recrystallization of ferrite in annealing treatment would not occur. The Hf added 9Cr ODS steel was composed of martensite and small amount of residual ferrite. The Y-Hf-O oxides in 9Cr-Hf steels included Y-Hf-O nanoclusters and $Y_2Hf_2O_7$. The increment order of refining effect of Ti, Zr and Hf on oxides in 9Cr ODS steel was Hf > Ti > Zr, and the strengthening effect of Hf on 9Cr ODS steels was superior to Ti and Zr. Al addition had a negligible improvement for the mechanical performance of 9Cr ODS steels, and meanwhile the ductility would be decreased.

*Keywords: Oxide nanoparticles, Spark plasma sintering, Carbides, Orientation relationship.*

# Unveiling the Re effect on microstructural stability, high-temperature strength of high-Cr CoNi-based superalloy

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## Abstract

In order to develop CoNi-based superalloys with superior comprehensive performance for blades in industrial gas turbine (IGT), the influence of Re on the coarsening of γ′ precipitates mechanism and mechanical properties at 950°C of high-Cr CoNi-based superalloys with different Re addition (0Re, 0.5Re and 1Re in at.%) was investigated, with the help of high-temperature X-ray diffraction (XRD) and atom probe tomography (APT) analysis. The results show that the addition of Re reduces the coarsening rate of γ′ phase, decreases the γ/γ′ lattice misfit and increases the degree of γ/γ′ segregation of almost all elements of the alloy. As a result, two key factors that have an effect on coarsening rate reduction of the γ′ phase were identified. Firstly, the addition of Re increases the degree of segregation of the "coarsening control element Cr" and its interfacial concentration gradient of Cr. Secondly, it reduced the lattice misfit and the interfacial energy of γ/γ′ phases. In terms of mechanical properties, the addition of Re increases the compression yield strength and reduces the minimum compression creep rate of the alloys at 950°C. This could be mainly attributed to the inversion of the W partitioning from γ matrix to γ′ precipitates over the addition of the Re element, which increased the strength of the γ′ phase.

*Keywords: CoNi-based superalloys, Rhenium-effect, microstructural stability, coarsening, mechanical properties.*

# Revealing the Microstructural Evolution and Strengthening Mechanisms of Additively Manufactured Ni-based Hastelloy X Superalloy

**Seung-Chang Han[1]**, Woo-Sung Kim[2], Tea-Sung Jun[1]

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## Abstract

Additive manufacturing (AM) of metals results in the formation of intricate and hierarchical dislocation structures due to the rapid cooling rates and cyclic heating/cooling cycles inherent in the manufacturing process. The thermal environment of additive manufacturing also includes steep thermal gradients and repetitive heating by the tracking laser, contributing to the emergence of intricate, non-equilibrium microstructures and diverse material properties. Additionally, the microstructure developed in additively manufactured Ni-based alloys has exhibited the presence of metastable cellular structures within grain boundaries. Despite the significant interest in additive manufacturing, the mechanisms underlying solidification and the formation of dislocation substructures and solidification rates remain inadequately understood.

In the present study, the mechanical properties of SLM-fabricated HX were investigated with respect to their dependence on post heat treatment. Subsequent solid solution heat treatment (SHT) and hot isostatic pressing (HIP) was performed, and their effects on the microstructure and mechanical behavior were examined. The results indicate that anisotropy is significantly reduced through recrystallization during post-heat treatment. To gain a better understanding of the evolution of dislocation cell structures during processing and heat treatment, mesoscale analysis was conducted to investigate the impact of non-equilibrium dislocation cells on mechanical behavior. Fundamental mechanisms differing the dislocation density and residual strain will be discussed with regards to dislocation plasticity.

*Keywords: Hastelloy X, (HR)EBSD, Mechanical properties, Heat Treatment, Selective laser melting (SLM)*

# Technical **Oral Session _ Session 9**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 9 (D9)** **16:00 -17:45, Nov. 22**

Chair : Jong-Taek Yeom (Korea Institute of Materials Science, Yoko Mitarai, University of Tokyo) Samda Hall A, 3F

16:00-16:30 **K-D1066** **[Keynote] Low-density, high-strength metal mechanical metamaterials beyond the Gibson-Ashby model**
Ma Qian (RMIT University, Australia)

16:30-16:45 **O-D0652** **Stable strain hardening mechanism of Ti-4Al-5Mo-5V-5Cr-1Nb alloy during room temperature compression**
Chuanyun Wang (Northwestern Polytechnical University, China)

16:45-17:00 **O-D0289** **The study of crack initiation of Ti-6Al-4V alloys subjected to dwell-fatigue loadings through high resolution digital image correlation**
HAO-YU HU (The University Of Tokyo, Japan)

17:00-17:15 **O-D0233** **Temperature dependence of deformation and fracture in a beta titanium alloy of Ti-22V-4Al**
Rei Yano (Kyushu University, Japan)

17:15-17:30 **O-D0510** **Globularization behavior of the lamellar alpha in Ti-17 alloy and its effect on mechanical properties**
Jianwei Xu (Northwestern Polytechnical University, China)

17:30-17:45 **O-D0197** **Investigation of kink band formation mechanism on layered α/β two-phase Ti-9Cr alloy with CPFEM simulations**
Junyu Zhu (University Of Tokyo, Japan)

# Low-density, high-strength metal mechanical metamaterials beyond the Gibson-Ashby model

**Ma Qian**[1], Haozhang Zhong[2,1], Raj Das[1], Jianfeng Gu[2]

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## Abstract

Low-density, high-strength, ductile metal mechanical metamaterials are in high demand for engineering applications but remain out of reach by the Gibson-Ashby model. Here we demonstrate a new design concept based on a generalized theoretical model or an extended Gibson-Ashby model to overcome this challenge. We show that the deformation mechanism of a strut-based metal lattice material depends on its strut length-to-diameter ($\ell/d$) ratio, and the key to maximizing its strength is to reduce its $\ell/d$ ratio to the minimum manufacturable level without increasing the lattice density. Inspired by this design concept, we investigate three strut remodeling strategies to strengthen metal lattices. Our low-density (1.6 g/cm$^3$) Ti-6Al-4V lattices designed according to Wolff's law of bone remodeling achieve exceptional strength (>400 MPa) compared to all cellular metallic materials of equivalent density reported so far (2-8 times their strength). Our $\ell/d$-centered design concept is expected to inspire the design of more metal metamaterials.

*Keywords: Metal Metamaterials, Lattice Materials, Strength, Density, Additive Manufacturing*

# Stable strain hardening mechanism of Ti-4Al-5Mo-5V-5Cr-1Nb alloy during room temperature compression

**Lianyang Chen**[1], Qiong Deng[1], Chuanyun Wang[2], Hongchao Kou[2], Jinshan Li[2]

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## Abstract

Strain hardening is crucial to the formability and reliability of structural materials, however, such important capacity will be rapidly reduced after yield until exhausted as strain increases. In current work, a stable strain hardening character is found in the compression of Ti-4Al-5Mo-5V-5Cr-1Nb alloy up to 40% strain, which can keep above 1000MPa. Microstructural characterization on deformed samples reveals the development of multiscale α'' lath frame. The stable strain hardening behaviour is understood via unveiling the roles of α'' lath during deformation. It is noted that these α'' laths impede dislocations and reduce their mean free path as strain increases. Meanwhile, a high density of dislocations can be observed within these nanoscale α'' laths, indicating they are also involved into deformation. Such a strain accommodation mechanism greatly reliefs the stress concentrated at β/α'' interfaces enabling the resistance to crack initialization. Molecular dynamics revealed the evolution process of martensitic transformation, indicating that the transformation of α'' can be activated when the atomic shear strain reaches 22.5%

*Keywords: strain hardening; metastable β titanium alloy; martensitic transformation; dislocation mean free path*

# The study of crack initiation of Ti-6Al-4V alloys subjected to dwell-fatigue loadings through high resolution digital image correlation

**Haoyu Hu**[1], Fabien Briffod[1], Takayuki Shiraiwa[1], Manabu Enoki[1]

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## Abstract

Although decades of studies have recognized substantial reduce in fatigue life due to load hold at high stress levels in near-α titanium alloys, the crack initiation mechanism in near-α titanium alloys under dwell-fatigue loadings is currently a topic of debate. The Stroh model involving strain redistribution at soft-hard grain/macrozone boundaries was pointed out as a possible mechanism for crack initiation of dwell-fatigue. Also, some other research showed the pre-defined strain localization at slip bands could be crack initiation sites. Besides, most recent research demonstrated possible crack initiation at twist boundaries of α-grains. Therefore, empirical evidence is highly desired to validate these models. To achieve this, the sub-grain scale in-plane deformation was assessed by ex-situ high-resolution digital image correlation (HR-DIC) analysis. In detail, flat specimens made from Ti-6Al-4V alloys were subjected to trapezoidal loadings with load hold of 120s at peak stress level. Several interruptions were designed for surface observations. Along with crystallographic information obtained from electron back-scattered diffraction (EBSD), transgranular slip bands with high strain localization, termed as slip damages, were found at three sites: (1) at triple points, (2) at high Schmid factor slip bands, and (3) at phase boundaries. Several cracks were identified on some of the slip damage sites. Out-of-plane deformation was also investigated by laser scanning confocal microscopy (LSCM). The results showed that cracks mostly initiated at slip damage sites with lower out-of-plane deformation components. Besides, although both slip damages and cracks seemed to be independent of macrozones, cracks tended to propagate fast within macrozones.

*Keywords: Ti-6Al-4V alloys, High resolution digital image correlation, Crack Initiation, Macrozone*

# Temperature dependence of deformation and fracture in a beta titanium alloy of Ti-22V-4Al

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## Abstract

Impact tests and tensile tests were conducted in the beta titanium alloy of Ti-22V-4Al between 77 K and 450 K to elucidate the temperature dependence of impact-absorbed energy, yield stress, effective shear stress, and activation volume. The impact-absorbed energy decreased with decreasing test temperature, however, this alloy did not undergo low-temperature embrittlement although it has a bcc structure. Tensile tests showed changes in both the work-hardening rate and the temperature dependence of yield stress at approximately 120 K. These suggest a change in the mechanism behind the plastic deformation at the temperature. The temperature dependence of the activation enthalpy for dislocation glide suggests that double-kink nucleation of a screw dislocation is the dominant mechanism for the dislocation glide from 150 K to 200 K, while the interaction between a dislocation and solute atoms dominantly controls the dislocation glide above 200 K. Stress-strain curves show that the superelasticity appears below 120 K at the yielding, suggesting that the yielding is governed by transformation-induced plasticity at the temperature range. The enhancement of toughness at low temperatures in these alloys is discussed from the viewpoint of dislocation shielding theory in order for the suppression of low-temperature embrittlement.

*Keywords: dislocation glide; thermally activated process; brittle-to-ductile transition; β titanium alloy; transformation-induced plasticity*

# Globularization behavior of the lamellar alpha in Ti-17 alloy and its effect on mechanical properties

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**Abstract**

Control method of globularization of the lamellar alpha for Ti-17 alloy and its effect on mechanical properties are investigated in this paper. For this purpose, hot compression and heat treatment tests are conducted in the two-phase field. The results indicate that globularization process is determined by deformation degree, heat treatment temperature and time, but it is independent on deformation temperature and rate. The globularization friction increases with the increasing deformation degree, heat treatment temperature and time. Microstructural observations suggests that the globularization process can be divided into two distinct stages. The first is the fast stage which occurs in the initial stage of heat treatment, and the second is the slow stage which includes microstructure changes in the mid and later stage of heat treatment. The first and slow stages are controlled by boundary splitting and microstructure coarsening, respectively. A kinetics model coupling strain and time is developed by introducing the intermediate parameter t0.5 in the framework of the JMAK model. The globularization fraction under different conditions are predicted based on this kinetics model. The results show a good agreement between experiment and prediction. In addition, the globularization of alpha lamellae has a significant impact on mechanical properties. The globularization is beneficial to tensile strength and plasticity for Ti-17 alloy. However, fracture toughness exhibits a decreasing trend as the increasing globularization fraction..

*Keywords: titanium alloy, globularization, mechanical properties.*

# Investigation of kink band formation mechanism on layered α/β two-phase Ti-9Cr alloy with CPFEM simulations

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## Abstract

Deformation kink bands were found in a layered α/β Ti-9Cr alloy after uniaxial compression tests. The metastable Ti-9Cr alloy was developed with a controlled thermomechanical process to decrease the dislocation mean free path in the β phase and obstruct the softer deformation mechanisms. According to its plastic anisotropy, such a structure could be more favourable for deformation kink. In this study, the effect of alternative stacking α/β layers on the kink deformation mechanism was examined with nanoindentation tests and simulated with Crystal Plasticity Finite Element Simulation Method (CPFEM).

The mechanical properties of the Ti-9Cr alloys were investigated with uniaxial compression tests. Nanoindentation tests were carried out to check the resultant strengthening. CPFE nanoindentation simulations were then conducted considering the measured crystal orientation and the CP parameters were calibrated to match the experimental load curves. Based on the understanding of the kink band formation in tested alloys, a phenomenological crystal plasticity model was developed that includes kinking to reproduce the mechanical response of the layered structure.

During uniaxial compression tests, pronounced deformation kink bands formation was observed. The rank-1 connection was tested and validated for the formed kink bands. The resultant strengthening caused by the formation of the deformation kink was found in the α phase titanium. Nanoindentation tests were conducted in multiple areas and EBSD analyses of these regions were performed. With calibrated CP parameters, the formation of the deformation kink bands was reproduced in the CPFEM software Abaqus.

*Keywords: Titanium alloy, Kink deformation, Plastic deformation, Mechanical properties, Crystal plasticity*

# Technical **Oral Session _ Session 9**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 9-1 (E9-1)** — **16:00 -18:40, Nov. 22**

**Chair :** Zhang Baicheng (University of Science and Technology Beijing) — Halla Hall B, 3F

16:00-16:30 **K-E1139** **[Keynote] Mechanical behavior of titanium lattice structures fabricated by powder bed fusion**
Laichang Zhang (Edith Cowan University, Australia)

16:30-16:50 **I-E0434** **[Invited] Microscopic phase separations in BioHEA fabricated by laser powder bed fusion**
Daisuke EGUSA (The University of Tokyo, Japan)

16:50-17:05 **O-E0015** **Precipitation of Al-Cu-Mg based composites produced by additive manufacturing**
Jiehua Li (Montanuniversität Leoben, Austria)

17:05-17:20 **O-E0207** **Characterisation of reused AlSi7Mg powder**
James Warner (The University of Sydney, Australia)

17:20-17:35 **O-E0324** **Alloy Design for Additive Manufacturing of High-Fraction γ′ Superalloys and the Resulting Changes in Microstructure and Mechanical Properties**
CHANHEE LEE (Changwon National University, Korea)

17:35-17:50 **O-E1119** **Warpage of thin-wall cantilever beam in selective laser melting process: experimental and inherent strain method modelling**
Chen Wang (Singapore Institute of Manufacturing Technology (SIMTech), A*STAR Research Entities, Singapore)

17:50-18:05 **O-E0296** **Controlling microstructure of additive manufactured Al-Si eutectic alloys based on computational thermal-fluid dynamics simulation**
Masayuki Okugawa (Osaka University, Japan)

18:05-18:20 **O-E0451** **Bio-additive manufacturing for control of bone matrix microstructure**
Aira Matsugaki (Osaka University, Japan)

18:20-18:40 **I-E0603** **[Invited] Study on PBF Additive Manufacturing Process and Characterization using Non-Spherical Hydrogenation-Dehydrogenation Titanium Powder**
Bin Lee (Kyung Hee University, Korea)

# Mechanical behavior of titanium lattice structures fabricated by powder bed fusion

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## Abstract

Lattice structures (Periodic cellular materials) are a type of architectures constructed by an array of spatial periodic unit cells with edges and faces. Although lattice structures exhibit a range of superior properties, such as low elastic modulus, high specific stiffness and strength, large surface area, a large number of internal pores, and relatively low-stress level, the manufacturing by traditional technologies and the optimization of properties of lattice structured are limited because of poor control over the morphological characteristics of the pore network. The recent advances in metal additive manufacturing (AM) technologies have enlarged the design and manufacturing possibilities for lattice structures, which provides lattice structures with promising solutions for a variety of applications. This work presents the recent progress of additive manufacturing and enhanced mechanical and catalytic performance of lattice structures. The selective laser melting (SLM) produced and electron beam melting (EBM)-produced beta-type biomedical titanium lattice structures, as potential load-bearing implants, demonstrate excellent mechanical properties in terms of high super-elasticity, low Young's modulus and high compression strength, high energy absorption and fatigue properties.

*Keywords: Additive manufacturing; Titanium; Lattice structure; Mechanical behavior; Fatigue*

# Microscopic phase separations in BioHEA fabricated by laser powder bed fusion

**Daisuke Egusa**[1], Ryosuke Ozasa[2], Masayuki Okugawa[3], Taisuke Sasaki[4], Takuya Ishimoto[5], Yuichiro Koizumi[6], Takayoshi Nakano[7], Eiji Abe[8]

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## Abstract

High entropy alloys (HEA) have attracted attention as a new class of structural materials. In particular, Ti-Zr-Nb-Ta-Zr alloys have been attracted as HEA for biomedical applications (BioHEA) due to their superior mechanical properties and biocompatibility than conventional Ti-based alloys. Recent studies reported that BioHEA fabricated by laser powder bed fusion (L-PBF), which enables ultra-rapid cooling, exhibits a nearly homogeneous microstructure at the microscopic scale. In HEA, multi-element disordered solid solution states are considered to be an important factor for their excellent properties, but the details have not been clarified. In this study, we have investigated microstructures of BioHEA fabricated by the L-PBF method (L-PBF BioHEA), based on X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), and three-dimensional atom probe (3DAP) for clarifying their influence on the excellent properties. XRD analysis revealed that L-PBF BioHEA consists of two bcc phases with slightly different lattice constants. STEM observations showed that the alloy has columnar crystal grains elongated along the building direction, accompanied by a submicron-scale cellular microstructure. Based on STEM-EDS and 3DAP analysis, we found that the composition is slightly different across the cell boundaries, corresponding to the two-phase separation identified by the XRD analysis. The observed phase separation phenomena can be explained according to solute partitioning trends in solidification during rapid cooling, based on thermodynamic calculations. The submicron-scale cellular microstructure is introduced to accommodate strains derived from phase separation behaviour by L-PBF fabrications, which contributes to the high strength of the BioHEA.

*Keywords: high entropy alloys (HEA), laser powder bed fusion (L-PBF), X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), three-dimensional atom probe (3DAP).*

# Precipitation of Al-Cu-Mg based composites produced by additive manufacturing

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## Abstract

Al-Cu-Mg based alloys (i.e. 2024 alloy) have been widely used in aerospace industry due to their high strength and light weight. However, Al-Cu-Mg based alloys have a significant hot tearing tendency and a serious segregation issue due to their large solidification range. An effective grain refinement can be used to solve the hot tearing and segregation issues. Although the addition of 0.1 wt.% TiB2 (as grain refiner) into Al-Cu-Mg based alloys (regarded as Al-Cu-Mg based composites) can refine grain size down to 200 μm, it is still not enough. In this paper, the addition of 3 wt.% TiB2 (as grain refiner) into Al-Cu-Mg based alloys will be investigated, which can refine grain size down to 50 μm and thereby greatly reduce hot tearing tendency and segregation. Furthermore, additive manufacturing (laser powder bed fusion) was used to produce rods with a diameter of 12 mm and height of 200 mm. The precipitation of Al-Cu-Mg based composites produced by additive manufacturing was also investigated by using transmission electron microscopy (TEM) and atom probe tomography (APT). Three different types of precipitates (Al-Cu (θ) phase, Al-Cu-Mg-Ag (Ω) phase and Mg-Si (β) phase) were observed, which is fully consistent with the case of samples produced by conventional gravity die casting condition. More interestingly, one Mg, Ag-rich layer was observed in the vicinity of Al-Cu (θ) phase. These careful TEM characterizations and quantitative atom probe data analyses give us some hints to design high performance Al-Cu-Mg based composites.

*Keywords: Al alloys, Precipitates, Additive manufacturing, TEM, APT*

# Characterisation of Reused AlSi7Mg Powder

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## Abstract

Additive manufacturing provides an excellent means of producing parts of complex geometries while maintaining an efficient use of resources due to its additive rather than subtractive nature. One of the most prevalent additive manufacturing technologies is powder bed fusion, especially in regard to the processing of metals.

In powder bed fusion, this efficient utilisation of resources relies on powder reuse, involving collecting and sieving any powder leftover from a given build to be used in subsequent processing. However, the powder bed fusion process and post process handling procedures change the properties of powder by the production of spatter particles and the creation and breakdown of agglomerate particles, among other processes. These will change the properties of the powder batch as a whole and so powder characterisation is required to understand the extent to which powder changes during the powder bed fusion process, to determine its usability for subsequent production runs. This is especially important regarding a powders ability to spread in the build chamber, as this will affect the quality of finished parts.

This work utilises a refreshing powder reuse strategy to investigate the effects of powder reuse on the flow properties, size, and morphology of AlSi7Mg powder in a laser powder bed fusion process. By investigating the Hall flow times, avalanche angle, powder cohesion, and size and shape measurements, AlSi7Mg powder is shown to change with continual reuse, even with the regular introduction of unused powder.

*Keywords: Additive manufacturing, Powder bed fusion, Powder reuse*

# Alloy Design for Additive Manufacturing of High-Fraction γ´ Superalloys and the Resulting Changes in Microstructure and Mechanical Properties

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## Abstract

Ni-based superalloys, recognized for their high-temperature strength, creep resistance, and corrosion resistance, are commonly utilized in gas turbine vanes and blades. This research investigates the electron beam melting (EBM) additive manufacturing process for René 80 superalloy, which contains over 40% γ' phase. In order to optimize the alloy composition and EBM process parameters, the study involved reducing the Ti content from 5 to 3 wt%, adding 2.5 wt% Ta, and introducing 1.0 wt% Hf to the alloy. These adjustments resulted in improved manufacturability, fewer defects, and enhanced high-temperature strength. The manufactured material demonstrated an increased γ' phase fraction, leading to better properties than those found in traditional cast samples. This study highlights the potential of EBM in manufacturing high-performance Ni-based superalloys for gas turbine applications, offering an alternative to conventional casting techniques. The optimized process parameters and alloy composition ensure that the resulting material exhibits the desired mechanical and thermal properties necessary for use in demanding high-temperature environments.

*Keywords: Ni-based superalloys; Additive manufacturing; Electron beam melting; Alloy design;*

# Warpage of thin-wall cantilever beam in selective laser melting process: experimental and inherent strain method modelling

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## Abstract

Additively manufactured structures produced via selective laser melting (SLM) process have gained significant prominence as a means to achieve net-zero manufacturing. However, challenges associated with thermal distortion and warpage have persisted within the SLM process due to the presence of high residual stresses during both the building and cooling phases. Such dimensional errors limit further adoption of additive manufacturing in industry to build large-scale and thin-wall geometries. While extensive studies focused on complex and coupled effects of process parameters on thermal distortion of SLM parts, the challenge in this work consists of corelating recoater orientation, air-flow direction and geometry factors with residual stress and warpage. Experimental investigations were conducted using the EOS M290 SLM machine to print a series of stainless steel cantilever beams along the X and Y coordinating axes. Subsequent wire-cutting procedures were employed to achieve specific thickness variations. The quantification of warpage was performed through precision measurements using a coordinate measuring machine (CMM). As results, a distinctive recoat-induced distortion was observed when beam thickness is less than 1.25 mm. It was apparent that the recoating system profoundly influenced the residual warpage within the SLM process, necessitating careful consideration of the part's orientation concerning both the recoating procedure and the direction of air flow. The study also developed warpage prediction model via inherent strain method. Results showed that inherent strain calibration under certain process parameters is not applicable for the cases affected by recoating direction and thin-wall geometries.

Keywords:
*Keywords: Selective beam melting; Inherent strain method; Thermal distortion; Residual stress; recoating direction; thin-wall cantilever beam*

# Controlling microstructure of additive manufactured Al-Si eutectic alloys based on computational thermal-fluid dynamics simulation

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## Abstract

Additive manufacturing (AM) has garnered substantial attention owing to its capability to fabricate parts with complex shapes. In addition, the powder-bed fusion (PBF) type AM process can also control internal microstructures through variations in process parameters. Microstructures of metals fabricated by the PBF process are solidification microstructures, and the solidification maps based on Hunt's columnar-equiaxed transition criterion are proposed as a guide for determining a process condition. On the other hand, we previously reported that the rapid heating condition during the melting process also affects the microstructure formation in Al-Si eutectic alloy, in which the solid-Si particles with high melting temperature remained after the rapid remelting act as heterogeneous nucleation sites during subsequent resolidification [Okugawa et al., J. Alloys Compd. 919 (2022) 165812]. However, the relationship between the melting conditions and the process conditions is unclear and is required to be revealed for obtaining the desired microstructure in the PBF process of the eutectic alloy. In this study, we investigated melting and solidification conditions in the PBF process of Al-Si eutectic alloy by laser-irradiation experiments and corresponding computational thermal-fluid dynamics simulations. It was found that the heating rates in the PBF process of Al-Si alloy are around $10^8$ K $s^{-1}$ and are 10 times higher than the cooling rates. The remaining Si particles in the remelting process are caused not only by the fast cooling but also by the significantly large heating rates in the PBF process.

*Keywords: Al-Si hypoeutectic alloy, Additive manufacturing, Laser powder bed fusion, Computational thermal-fluid dynamics (CtFD) simulation*

# Bio-additive manufacturing for control of bone matrix microstructure

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## Abstract

Bio-additive manufacturing is an innovative technology that enables the construction of various kinds of living tissues by building up biological cells as well as biochemical molecules. The replacement of the damaged tissue and organs with the created bio-mimetic structures allows for the accelerated recovery of their intrinsic functions. In particular, the generation of bone-mimetic microstructures with the anisotropic texture of collagen/apatite is imperative for bone tissue regeneration. Bone matrix texture formation is dominantly regulated by the unidirectional arrangement of osteoblasts, which is genetically controlled under three-dimensional mutual communication among the cells. In this study, a three-dimensional bone-mimetic anisotropic microstructure was successfully obtained by the bio-additive manufacturing method using the laminated layer method of oriented collagen scaffold. Unidirectional osteoblasts arrangement was artificially controlled by the scaffold molecular design through integrin signaling. Prolonged culture allowed for the differentiation of osteoblasts into osteocytes along with the ordered bone matrix texture formation. The cells and matrix maturation further constructed the ordered osteocyte networks inside the bone matrix, indicating that the bio-additive manufacturing process realized the biological process of bone differentiation and functionalization even outside the body. Moreover, recent studies have shown the remarkable results of cellular activation using metal additive manufacturing materials. The results open future perspectives for customized bone medical device development and also help bone organoid research development.

*Keywords: Bio-additive manufacturing. Biological tissue, Bone matrix microstructure, Cell arrangement, Biomedical device*

# Study on PBF Additive Manufacturing Process and Characterization using Non-Spherical Hydrogenation-Dehydrogenation Titanium Powder

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**Abstract**

Metal powder bed fusion (PBF) additive manufacturing has entered commercialization in areas such as medical, defense and aerospace due to its high design freedom and ability to produce custom parts without the need for molds. However, expensive spherical powders are mainly used to ensure spreadability and flowability, making it difficult to penetrate industries such as electronics and personal transportation devices due to high material costs. In this study, we investigated the improvement of powder flow properties and the PBF additive manufacturing process using low-cost hydrogenation-dehydrogenation (HDH) titanium(Ti) powder.

The introduction of a hydrophobic surface treatment process significantly improved the powder flow characteristics to a level suitable for PBF processing. A 1:1 mixture of spherical Ti powder and surfaced treated HDH Ti powder was then used in the PBF additive manufacturing process. After annealing at 650 ℃ for one hour, we successfully produced parts with a tensile strength of 924 MPa and an elongation of 9.5%. Due to the high oxygen content in the HDH Ti powder, it has higher strength and lower elongation compared to the typical mechanical properties of Ti parts. However, considering that the non-spherical powder is only about 10% of the price of spherical powder, this study significantly reduces the cost of the PBF additive manufacturing process.

*Keywords: Powder bed fusion, hydrogenation-dehydrogenation titanium powder, powder flow properties, spreadability*

# Technical **Oral Session _ Session 9**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 9-2 (E9-2)** **16:00 - 18:00, Nov. 22**

**Chair :** Jung-Wook Cho (Pohang University of Science and Technology) 201B, 2F

16:00-16:15 **O-E0115** **Nano-structured Fe-TiB2 high-modulus steel through direct energy deposition**
Renlong Xiong (Wuhan Institute of Technology, China)

16:15-16:30 **O-E0662** **The effect of preheating and feature size on crack formation with the focus on crystallographic texture: Pure chromium fabricated by laser powder bed fusion**
Ozkan Gokcekaya (Osaka Univeristy, Japan)

16:30-16:45 **O-E0239** **Fundamental Characteristics of Three-Dimensional Additive Manufacturing Products of Zero Thermal Expansion Metal**
Nobuuyki Oyama (NIPPONCHUZO K.K., Japan)

16:45-17:00 **O-E1030** **Magnetic field assisting laser additive manufacturing**
Chaoyue CHEN (Shanghai University, China)

17:00-17:15 **O-E0956** **Development of 3D printers employing multiple molding methods and composite gel materials**
Tsubasa Honma (Yamagata University, Japan)

17:15-17:30 **O-E0727** **Nanomechanical investigations into the effects of hydrogen on the mechanical behavior of additively-manufactured alloy**
Yakai Zhao (Agency for Science, Technology and Research (A*STAR), Singapore)

17:30-17:45 **O-E0735** **Effect of Oxygen and Nitrogen on the Microstructure and Hardness of Ti-6Al-4V Fabricated by Laser Powder Bed Fusion**
Woohyeok KIM (HANBAT National University, Korea)

17:45-18:00 **O-E0200** **Superior cryogenic tensile strength of Carbides reinforced NiCoCrC medium-entropy alloy fabricated via additive manufacturing**
So-Yeon Park (Inha University, Korea)

# Nano-structured Fe-$TiB_2$ high-modulus steel through direct energy deposition

**Renlong Xiong**[1], Eunseong Kim[2], G.M. Karthik[3], Hyoung Seop Kim[4]

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**Abstract**

Lightweight structural materials are strongly demanded for saving energy consumption and better performance of machines and transportation systems. The key criterion to design these lightweight load-bearing materials are high stiffness (i.e. elastic modulus E), reduced mass density ρ, sufficient ductility, as well as high strength, i.e., yield strength (YS) and ultimate strength (UTS). However, these material properties are mutually exclusive. It is still a challenge to design materials with high specific stiffness (E/ρ), together with high strength-ductility synthesis. Here a nano-structured Fe-$TiB_2$ high-modulus steel (HMS) with enhanced strength and specific stiffness was successfully fabricated through direct energy deposition (DED). The results showed the Fe-$TiB_2$ HMS possessed a superior specific stiffness than most metals and alloys due to the induction of large amounts of $TiB_2$ particles with low mass density. In addition, the DED sample annealed at 800 °C for 1 hour also presented a high YS and UTS of 702 MPa and 1252 MPa, respectively, yet maintained a good ductility of 8.2%. This could mainly be attributed to the heterogeneous structure that the hard nano-$TiB_2$ particles inside the soft ferrite were evenly distributed along the grain boundary.

*Keywords: Direct Energy Deposition; High-modulus Steel; $TiB_2$; Elastic Modulus; High Strength*

# The effect of preheating and feature size on crack formation with the focus on crystallographic texture: Pure chromium fabricated by laser powder bed fusion

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[Introduction] Chromium (Cr) metal has attracted significant attention as an alloy system since the late 1950s because of its higher melting point (1863 ºC), lower density, and higher thermal conductivity as a candidate for high-temperature applications. However, the use of Cr metal has been impeded due to its high ductile-to-brittle transition temperature (DBTT), which is approximately 150 ºC for pure Cr. Below the DBTT, pure Cr exhibits a brittle behavior and exhibited severe cracking. Since LPBF is featured by its flexible shaping ability, it has been utilized for the fabrication of a variety of products with complicated three-dimensional structures. Moreover, LPBF is suitable for near-net-shape processing of difficult-to-process materials, and its application to such metal materials has begun to be tested. However, it is challenging to fabricate pure Cr by laser powder bed fusion (LPBF) due to high cooling rate. To overcome the limitations, the Cr microstructure should be tuned to resist cracking during the LPBF process. This study focused on crystallographic texture and related grain boundary characteristics distribution (GBCD) of LPBF-processed pure Cr to avoid cracking with help of an increase in base temperature and shorter scan area. Recent studies have shown that the LPBF process is highly effective in controlling the crystallographic texture of various metallic materials, from randomly oriented polycrystalline to single crystalline-like microstructures, and the resulting enhanced structural and functional properties. Considering the advantage of layer-by-layer fabrication of the LPBF process forming epitaxial growth and promoting crystallographic texture, it is expected to tune GBCD and prevent crack initiation and propagation. Because it is clarified in our previous study that cracks in Cr follow a high-angle grain boundary (HAGB) which can be eliminated by single-crystal-like texture formation.

[Experimental] An LPBF machine (EOS M290, Munich, Germany) equipped with a 400 W Yb laser was used to manufacture the pure Cr specimens with dimensions of 10 × 10 × 5 mm and 5 × 5 × 5 mm along the x-, y-, and z-axes, respectively. Bidirectional laser scanning was performed under an Ar atmosphere with a rotation of 90° between layers (XY scan). The baseplate was preheated to 80°C to up to 200°C. As-built specimens were analyzed by optical microscopy (OM), and scanning electron microscopy (SEM) equipped with electron back scattering (EBSD). To evaluate mechanical properties, Vickers hardness and compression tests were carried out.

[Results] In this study, two different approaches were applied to tune the microstructure, which are preheating and feature size. High baseplate temperature and smaller feature size exhibited strengthening in crystallographic texture, resulting decrease in HAGB density, as a result, crack density was decreased. The crack-resistant Cr exhibited improved mechanical properties under compression. Thus, strengthening crystallographic texture via preheat or feature size is a promising approach to prevent severe cracking in hard-to-process materials and enhance the density.

# Fundamental Characteristics of Three-Dimensional Additive Manufacturing Products of Zero Thermal Expansion Metal

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## Abstract

Demand for low thermal expansion materials is increasing due to the electrification of automobiles and the increase in communication volume. Furthermore, products that have high thermal conductivity as well as low thermal expansion properties have been earnestly desired in recent years.

Metal additive manufacturing technology has made it possible to manufacture products having complicated shapes. However, there are still few reports of additive manufacturing technology using low thermal expansion materials.

The authors report the basic research results for the purpose of developing additive manufacturing technology for low thermal expansion metals. As a result, it became possible to improve the physical properties and reduce the weight by applying additive manufacturing technology to the low thermal expansion material. In addition, a complicated shape can be manufactured at a lower cost than a simple block product.There was no anisotropy in various physical properties of the SLM products, and no secular change in dimensions and coefficient of thermal expansion was confirmed. There is no significant difference in machinability between SLM products, cast products and forged products. Therefore, it is considered that SLM products can be used in the same manner as conventional cast steel products.

Furthermore, as an application example of the technology, we will introduce complicated and lightweight products.

*Keywords: Additive manufacturing, Low thermal expansion metal, SLM, Weight saving*

# Magnetic field assisting laser additive manufacturing

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## Abstract

Although laser additive manufacturing technology can prepare high-performance metal materials, there are still various problems such as strong texture, residual stress, anisotropy of mechanical properties, and low plasticity caused by extremely high cooling rates and temperature gradients. In order to realize the microstructure and performance control of additive manufacturing high-performance alloys, the team of Shanghai University proposed the Magnetic Assisting Additive Manufacturing (Magnetic Assisting Additive Manufacturing, MAM) technology. The comprehensive mechanical properties of the prepared Ti6Al4V and Al12Si alloys are significantly better than the current advanced level, effectively solving the problem of microstructure control of metal materials prepared by LMAM, and ensuring the development of multiple key components in the aerospace field. This report will show the research progress of the Shanghai University team in recent years in the fields of magnetic field-controlled laser additive manufacturing molten pool flow and heat transfer, solidification structure, residual stress metallurgical defects, and comprehensive mechanical properties.

*Keywords: Magnetic field, Laser additive manufacturing, microstructure, mechanical properties.*

# Development of 3D printers employing multiple molding methods and composite gel materials

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## Abstract

Various methods of 3D gel printers have been reported for fabricating on-demand flexible structures such as 3D cell scaffolds and soft robots. 3D gel printers can fabricate hollow structures of arbitrary shapes, which is difficult to achieve by molding. On the other hand, most 3D gel printers have been based on a single method, and it has been difficult to incorporate multiple gel materials with different mechanical properties into a single object. Therefore, we have developed a 3D gel printer GelPiPer-multi that employs both SLA (Stereo Lithography Apparatus) and DIW (Direct Ink Writing).

SLA is a molding method in which light-curing liquid resin is irradiated with a UV laser beam in the form of dots, and the resin is solidified one layer at a time and stacked. On the other hand, DIW is a 3D printing method that directly writes ink. In this study, these two methods were combined to create a composite gel. First, ink is stacked on the stage by DIW, and then cured by UV-LED irradiation. Next, the stage is lowered into a bathtub and cured by irradiating a UV laser from the top surface using the SLA method. This process is repeated to composite the gel material. In this study, we report on the GelPiPer-multi and the composite gel structure that was produced by the GelPiPer-multi.

*Keywords: 3D printer, Hydro Gels, Composite Materials*

# Nanomechanical investigations into the effects of hydrogen on the mechanical behavior of additively-manufactured alloy

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## Abstract

The microstructures of alloys additively manufactured (AM) using laser powder bed fusion or other laser-based technologies are distinct in several different ways, among which a key feature is the presence of an ultrafine solidification cellular structure with dense dislocations and often segregations and precipitations decorated. To experimentally explore how the AM alloys behave in hydrogen environments and especially the role of the unique cellular structures, a series of nanomechanical tests, including nanoindentation and micro-pillar compression, were conducted on the AM fabricated 316L stainless steel. The experimental results suggested that, compared to its conventionally manufactured counterpart, AM 316L shows lower apparent hydrogen diffusivity and a better resistance to hydrogen-induced strengthening. By conducting both direct low-load nanoindentation on the cell walls and micro-compression tests for cell-included pillars, the role of cellular structure in terms of hydrogen-affected mechanical behaviour is also revealed and discussed.

*Keywords: Nanoindentation; pillar compression; hydrogen embrittlement; additive manufacturing; stainless steel.*

# Effect of Oxygen and Nitrogen on the Microstructure and Hardness of Ti-6Al-4V Fabricated by Laser Powder Bed Fusion

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## Abstract

Components made of Ti-6Al-4V using additive manufacturing processes offer the advantage of producing complex-shaped parts with greater accuracy compared to conventional methods. As a result, they are widely utilized in various fields, including aerospace, biomaterials, and chemical plant industries. In the additive manufacturing process, Ti-6Al-4V ELI grade powder with a very low concentration of interstitial elements is commonly employed. However, there may be variations in the impurity content of the ELI powder depending on the processing conditions or manufacturer. This study aimed to investigate the microstructural changes and mechanical properties of Ti-6Al-4V samples produced through laser powder bed fusion (L-PBF) while varying the oxygen/nitrogen content. The microstructure of the components was analyzed using OM, SEM, and EBSD techniques, while XRD analysis was conducted to assess lattice parameter differences. Additionally, Vickers hardness measurements were taken to evaluate the mechanical properties. The results revealed that increasing the oxygen/nitrogen content in the powder led to higher porosity, while reducing the thickness of alpha laths and the size of prior beta grains. Furthermore, an increase in the oxygen/nitrogen content resulted in higher Vickers hardness. These findings seem to be attributed to the influence of interstitial elements such as oxygen and nitrogen on the atomic diffusion rate of the surrounding atoms, thereby refining the microstructure.

*Keywords: additive manufacturing, Ti-6Al-4V, selective laser melting, ELI powder, microstructure*

# Superior cryogenic tensile strength of Carbides reinforced NiCoCrC medium-entropy alloy fabricated via additive manufacturing

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## Abstract

A NiCoCr medium entropy alloy (MEA) is a promising MEA in which the Cantor (equiatomic CrMnFeCoNi) HEA is modified. A NiCoCr is reported to exhibit the best cryogenic mechanical properties due to the highest lattice misfit among Cantor system HEAs/MEAs. However, despite the superior properties of the MEA (like cryogenic impact toughness, radiation resistance, corrosion resistance, etc.), low room temperature strength and high price still make it difficult to commercialize. In this work, to further improve the mechanical characteristics of NiCoCr, 0.75 at.% carbon is added to a NiCoCr and tried to be fabricated using laser powder bed fusion additive manufacturing (AM) process. The observation of as-built specimens' microstructure showed that heterogeneous grain structure and epitaxial growth grains along the building direction. And a sub-structure decorated of a dislocation network and in-situ formed carbides during AM was observed inside the grains. In addition, post heat treatment was performed to relieve residual stress and increase the precipitate volume fraction. After the post heat treatment, some subgrains underwent partial recrystallization and the size and number of the precipitates was increased simultaneously. As the results of the cryogenic tensile test, for AM-built NiCoCrC MEA, the ultimate tensile strengths were 1.60 GPa and the yield strengths were 1.23 GPa. Interestingly, yield strengths of NiCoCrC were superior than that of cast NiCoCr MEAs and additively manufactured HEAs and evenly SUS 316LN alloy, the most representative alloy for cryogenic applications. The deformation behavior and fracture mechanism were also discussed in connection with results of microstructural features.

*Keywords: Laser powder bed fusion, NiCoCrC medium-entropy alloy, Nano-sized precipitate, Cryogenic tensile properties, Heterogeneous microstructure*

# Technical **Oral Session _ Session 9**

## **Symposium F :** Thin Films and Surface Engineering

**Thin Films and Surface Engineering 9 (F9)** **16:00 - 16:55, Nov. 22**

**Chair :** Jian He (Beihang University) 202A, 2F

16:00-16:20 **I-F0579** **[Invited] Research Progress of Laser Hybrid Surface Engineering**
Jianhua Yao (Zhejiang University of Technology, China)

16:20-16:35 **O-F1113** **Research on Surface Coating Technology of Zirconium Alloy Cladding for Nuclear Fuel Elements**
ZHANG RUIQIAN (Nuclear Power Institute of China, China)

16:35-16:55 **I-F1163** **[Invited] Advanced Metallization Technologies using atomic layer deposition (ALD) and area-selective ALD (AS-ALD)**
Soo-Hyun Kim (Ulsan National Institute of Science and Technology, Korea)

# Research Progress of Laser Hybrid Surface Engineering

**Jianhua Yao[1,2]**

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## Abstract

Laser surface engineering has the advantages including high flexibility, high quality and environmental friendliness, and have been widely used in energy equipment, mining machinery, metallurgical equipment, petrochemical industry and other fields. With the trend of diversification, on-site and high-quality in surface engineering, the laser manufacturing technology of single material, single performance and single energy field begins to develop towards composite materials, selection performance customization and multi-energy field assistance. As an important development direction and supplement of single laser technology, energy field assisted laser surface engineering can break through the bottleneck of single laser technology, and obtain more precise, more efficient and smarter processes. It will further promote the transform and upgrading of the manufacturing industry.

This report summarizes the research status of energy field assisted laser surface engineering around the world, and introduces the recent progress of the author's group on the manufacturing with laser/electromagnetic hybrid, laser/kinetic hybrid, laser/vibration hybrid and laser/electrochemical hybrid, etc. The advantages of laser hybrid manufacturing are analyzed in the aspects of material properties, microstructures and forming properties. The challenges and solutions on efficiency, performance, cost, and intelligence of the laser hybrid remanufacturing are discussed and analyzed from the perspective of fundamental study and industrial application. Finally, the future direction of the energy field assisted laser surface engineering is forecasted.

*Keywords: Laser surface engineering; laser hybrid manufacturing; energy field*

# Research on Surface Coating Technology of Zirconium Alloy Cladding for Nuclear Fuel Elements

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## Abstract

After the 2011 Fukushima nuclear accident in Japan, in order to prevent rapid failure of nuclear fuel components under accident conditions and reduce the risk of a large amount of radioactive material leakage, there was an international research boom on accident resistant fuel (ATF). Compared with traditional UO2 zirconium alloy system nuclear fuel, accident resistant fuel can improve the inherent safety of fuel elements under accident conditions, while maintaining or improving the performance of fuel elements under normal operating conditions. The plan of plating protective coatings on the surface of zirconium alloy cladding to improve the corrosion resistance and oxidation resistance of the cladding is expected to achieve engineering application in the short term. The China Nuclear Power Research and Design Institute (NPIC) launched research on surface coatings of zirconium alloys in 2016, and conducted basic research on coating composition and process in the early stage. Based on this, the zirconium alloy surface coating technology was focused on the PVD process to prepare metal Cr coatings, mastering the preparation process of Cr coatings on zirconium alloy surfaces, and developing representative engineering samples of zirconium alloys with Cr coatings, We have independently developed a prototype PVD system for preparing large-sized zirconium alloy surface coatings and mastered the preparation technology of metal Cr coatings on the surface of slender (4m) zirconium alloy tubes. We have conducted performance research on corrosion, mechanics, bonding behavior, high-temperature oxidation, friction and wear, thermal shock, irradiation, and other systems. The research results indicate that the Cr coating on the surface of the prepared zirconium alloy has a fine and dense microstructure, good bonding quality, and excellent service performance of the zirconium alloy cladding material after coating modification. It has been preliminarily applied in commercial nuclear power plants and will be gradually promoted and applied on a large scale in the future.

*Keywords: Zirconium Alloy Cladding , Nuclear Fuel Elements , PVD Coating, Corrosion, Irradiation*

# Advanced Metallization Technologies using atomic layer deposition (ALD) and area-selective ALD (AS-ALD)

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As the on-chip interconnect scales down continuously, it faces challenges in all aspects of performance of the present Cu interconnects. Performance degradation caused by electron scattering in narrow Cu damascene lines, combined with slow barrier/liner scaling is a big concern. In this presentation, advanced technologies based atomic layer deposition (ALD) and area-selective ALD (AS-ALD) are discussed to overcome the present problems of Cu internnects. Ru/ZnO bilayer grown by ALD is introduced as a multifunctional layer for advanced Cu metallization [1-4]. Here, ZnO as a diffusion barrier and glue layer is selectively grown on $SiO_2$ excluding Cu, and then Ru thin film as both a liner and seed layer is grown on both surfaces by ALD. Ru/ZnO bilayer can serve as multifunctional layer for advanced Cu interconnects and moreover, the formation of bottomless barrier by eliminating ZnO on via bottom, or Cu, via resistance is expected to be decreased for ever-shirking Cu line. We also discuss three fascinating options for Ru-ALD processes, which can be used in various applications, including logic interconnects to replace Cu, 3D NAND gates, metal gates, capacitor electrodes, seed layer/liner for Cu EP, backside power distribution (BSD) etc., are provided.

**References**

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*Keywords: atomic layer deposition, area-selective atomic layer deposition, Cu metallization, Ru, ZnO.*

# Technical **Oral Session _ Session 9**

## **Symposium G :** Materials for Energy Storage and Generation

**Materials for Energy Storage and Generation 9 (G9)** **16:00 - 17:00, Nov. 22**

**Chair** : Dong-Hwa Seo (Korea Advanced Institute of Science and Technology) 303A, 3F

16:00-16:30 **K-G1180** **[Keynote] Rational design of porous carbon composites for energy storage and conversion**
Hao Liu (University of Technology Sydney, Australia)

16:30-16:45 **O-G0960** **Non-dendritic Electrodeposition of Alkali-Metal Anodes by Solvation Structure Modification in Dual-Cation Electrolytes**
Hongyi Li (Tohoku University, Japan)

16:45-17:00 **O-G0975** **Facilitating Multivalent Cation Diffusion in Cathode Materials by Concomitant Intercalation in Dual-Cation Electrolytes**
YUE QI (Tohoku University, Japan)

# Rational Design of Porous Carbon Composites for Energy Storage and Conversion

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## Abstract

To survive from the coming energy crisis, many countries are concentrating attention once again on national initiatives to re-evaluate utilization of alternative energy sources and replacement of the internal combustion engine with a wireless electric motor. It is crucial, therefore, to develop new materials or technologies to improve the electrochemical performance of energy storage and conversion systems. Porous carbon based materials have been attracted great attention owing to their unique structures and electrochemical properties for energy storage and conversion.[1] Herein, we summarized relevant materials applied to a series of applications, including rechargeable batteries and electrocatalysts.[2-5] The results demonstrate that these porous carbon based materials exhibit excellent electrochemical performance owing to their unique properties. This contribution would be instructive for the enhancement of nanostructured materials for energy storage and conversion.

Reference

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*Keywords: Porous carbon, composites, rechargeable batteries, electrocatalysts, energy storage and conversion*

# Non-dendritic Electrodeposition of Alkali-Metal Anodes by Solvation Structure Modification in Dual-Cation Electrolytes

**Hongyi Li**[1] and Tetsu Ichitsubo[2]

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## Abstract

Alkali metals such as Li and Na are promising anode metals for rechargeable batteries because they possess the highest theoretical capacity. However, these alkali metals typically exhibit extremely rapid reaction kinetics during electrodeposition, resulting in a rapid depletion of the alkali cations close to the electrode surface. The intense concentration gradient of the alkali cation formed toward the electrode surface drives the dendritic growth of the alkali metals under a diffusion-limited condition.[1] The dendrites are weakly bonded and easily peels away into the electrolyte, which causes a significant loss of battery capacity and ignition risks.

To inhibit the unfavourable dendritic growth during electrodeposition, we constructed dual-cation electrolytes,[2-4] containing multivalent cations such as $Ca^{2+}$ and $Ba^{2+}$ as additives. The Coulomb interaction between the multivalent and monovalent cations modifies the solvation environment in the electrolytes. In particular, the $Li^{+}$ and $Na^{+}$ are encouraged to coordinate directly with the anions, forming contact ion pairs (CIPs) from the solvent-separated ion pairs (SSIPs). The formation of CIPs increases the desolvation energy of the alkali cations, thereby maintaining the electrodeposition under a reaction-limited condition and circumventing the dendritic growth. In addition, because the multivalent cations ($Ca^{2+}$, $Ba^{2+}$) are typically difficult to be reduced on the anodes and inserted into intercalation cathodes, the alkali cations ($Li^{+}$, $Na^{+}$) can be maintained as the sole carrier ions in the electrode reactions for constructing alkali metal anode batteries.

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*Keywords: rechargeable batteries, alkali metal anodes, dual-cation electrolytes, concerted effects, solvation structure modification, non-dendritic morphology.*

# Facilitating Multivalent Cation Diffusion in Cathode Materials by Concomitant Intercalation in Dual-Cation Electrolytes

**Yue Qi[1],** Hongyi Li[2], Tetsu Ichitsubo[3]

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## Abstract

Multivalent elements such as Mg and Ca are receiving significant consideration in the development of the next-generation rechargeable batteries. These elements are advantageous for reducing the production costs and improving the performance due to their abundance of sources and high theoretical capacity. Besides, compared to the alkali elements (Li or Na), the multivalent elements have a lower tendency for dendritic growth, which is preferable from a safety standpoint. However, developing suitable cathode materials for the multivalent elements presents numerous challenges. Due to the strong Coulomb interaction with the host structures, the multivalent cations exhibit typically sluggish kinetics and large overpotentials during intercalation into cathode materials, resulting in significant capacity degradation.[1]

To aid in the solid-state diffusion of the multivalent cations, we proposed a concept of dual-cation/dual-salt electrolyte systems,[2-4] in which the monovalent alkali cations serve as assistants. Using the spinel-type $MgCo_2O_4$ and Chevrel compounds $Mo_6S_8$ cathodes, we demonstrated that the $Li^+$ and $Mg^{2+}$ cations were concomitantly inserted into host structure, thereby increasing the discharge capacity and decreasing the overpotential.[3,4] Moreover, the first-principles calculations revealed that the concerted migration of $Li^+$ and $Mg^{2+}$ cations in the host structure significantly reduces the activation energy,[5] which is consistent with the overpotential decrease observed in the experiments. Furthermore, we investigated the intercalation behavior of $Mg^{2+}$ and various alkali cations ($Li^+$, $Na^+$, $K^+$) in hollandite-type α-$MnO_2$ cathodes, confirming the versatility and deriving the general rules for exploiting the concomitant intercalation behavior.

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*Keywords: multivalent cation batteries, dual-cation electrolytes, solid-state diffusion, concerted effects, alkali cation additives.*

# Technical **Oral Session _ Session 9**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 9 (K9)** **16:00 -17:40, Nov. 22**

**Chair :** Tetsu Ichitsubo (Tohoku University) Samda Hall B, 3F

16:00-16:20 **I-K0693** **[Invited] Surface modification of metallic glasses for functional applications**
Karam Lim (Korea Institute of Materials Science, Korea)

16:20-16:40 **I-K0181** **[Invited] Changes in atomic and electronic structures in a Gd65Co35 metallic glass by cryogenic rejuvenation**
Shinya Hosokawa (Kumamoto University, Japan)

16:40-16:55 **O-K1034** **Research and application of high-entropy alloys hard coatings**
Bing Yang (Wuhan University, China)

16:55-17:10 **O-K1009** **Combustion behavior of Cu46Zr46Al8 bulk metallic glass in oxygen-enriched environments**
Hui Wang (University of Science and Technology Beijng, China)

17:10-17:25 **O-K1144** **Discontinuous coarsening stabilizes excellent ductility in high-entropy alloys with different recrystallization volume fractions**
Yang Zhongsheng (Northwestern Polytechnical University, China)

17:25-17:40 **O-K1172** **TiZrHfNb refractory high-entropy alloys with twinning-induced plasticity**
Shubin Wang (Shanghai Jiao Tong University, China)

# Surface modification of metallic glasses for functional applications

**Ka Ram Lim[1],** Sang Tae Woo[1,2], Young Sang Na[1], Seoung Zeon Han[1]

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## Abstract

Research on metallic glass powders and ribbons as functional materials, including thermoelectric materials, shape memory alloys, and supercapacitors, has been actively conducted in recent years. Our study aimed to investigate the potential bactericidal properties of metallic glasses with high Cu content for functional applications. $Zr_{50}Cu_{50}$ metallic glass was selected due to its high Cu content, simple chemical composition, and good glass stability.

Typically, Zr-based metallic glasses have an amorphous zirconium oxide film that strongly inhibits further oxidation. However, surface defects can compromise the glass stability of the amorphous oxide film, leading to the formation of a thick natural oxide layer.

In this study, we demonstrated that the oxidation behavior of melt-spun $Zr_{50}Cu_{50}$ metallic glass foil was affected by the surface casting defects on the wheel side, leading to a significant improvement in antibacterial properties. The superior antibacterial properties of the wheel side were attributed to the metallic Cu islands exposed on the surface.

*Keywords: Metallic glass, antibacterial, oxidation, Cu, catalyst*

# Changes in atomic and electronic structures in a $Gd_{65}Co_{35}$ metallic glass by cryogenic rejuvenation

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**Abstract**

Rejuvenation in glasses is defined as an excitation to a higher energy state by an external stress. Ketov et al. reported a rejuvenation effect by a temperature cycling between room- and liquid $N_2$ temperatures [1]. Hufnagel reviewed such a cryogenic rejuvenation and suggested that non-affine deformation must be caused on an atomistic length scale [2].

Based on their suggestions, we carried out some element-selective structural experiments on a $Ga_{65}Co_{35}$ metallic glass (MG) and found distinct structural changes around both the Gd and Co atoms [3]. We also measured inelastic x-ray scattering (IXS) and an increase of the elastic heterogeneity is detected as an increase of the width of longitudinal acoustic excitation peaks in the IXS spectra [3]. Subsequently, we performed photoemission and inverse-photoemission spectroscopies experiments and found the remarkable changes in the valence- and conduction-band density of states as well as core-level states by the cryogenic rejuvenation.

In this paper, we will present the structural and electronic changes in the $Ga_{65}Co_{35}$ MG by the cryogenic rejuvenation in detail, and the intrinsic mechanism of the rejuvenation from the atomic and electronic structures and particle dynamics in this MG. We will also report similar behaviours in a $Ga_{65}Ni_{35}$ MG.

[1] S. V. Ketov et al., *Nature* **524**, 200 (2015).
[2] T. C. Hufnagel, *Nature Mater*. **14**, 867 (2015).
[3] S. Hosokawa et al., *Nature Commun*., submitted.

*Keywords: Rejuvenation Effect, Temperature Cycling, High-energy x-ray diffraction, Anomalous x-ray scattering, Electron spectroscopies.*

# Research and application of high-entropy alloys hard coatings

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## Abstract

High-entropy alloys are usually composed of five or more primary elements. Based on their unique high entropy effect, lattice distortion effect, hysteresis diffusion effect and cocktail effect, high entropy alloys exhibit properties of high hardness, high toughness and high temperature resistance that are superior to those of conventional alloys, and show great potential for application in the field of protective coatings. However, the research on high-entropy alloy coatings is still in the initial stage, and there is a lack of in-depth research on the structure and performance of the coatings. We prepared the metal, nitride, and oxide coatings around the AlCrNbSiTi high-entropy alloy system by magnetron sputtering and arc ion plating techniques, characterized the evolution of microstructure such as phase composition, grain scale, and orientation of the coatings, and conducted systematic tests on the mechanical properties, friction behavior, and temperature resistance of the coatings, explored the mechanisms of toughness and elemental coupling of the coatings We also explored the mechanism of coating toughness and elemental coupling, studied the wear loss behavior of the coating, and obtained the internal elemental diffusion law and oxidation mechanism of the coating at high temperature.

*Keywords: high-entropy alloys, hard coatings, physical vapor deposition, nanocomposite structure, mechanical properties.*

# Combustion behavior of Cu46Zr46Al8 bulk metallic glass in oxygen-enriched environments

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**Abstract**

The present work used a specially designed experimental apparatus with an in situ measurement system to study the combustion of a Cu46Zr46Al8 bulk metallic glass (BMG). This material exhibited more violent and much more rapid combustion compared with its crystalline counterpart. The combustion mechanism was explored by evaluating the associated thermodynamics and kinetics and the effects of various crucial factors on the combustion behavior. The present findings improve our understanding of the combustion mechanisms of metastable metallic materials and also provide guidelines for the development of novel BMGs as advanced energetic materials.

*Keywords: Amorphous alloys; Melting; Oxidation*

# Discontinuous coarsening stabilizes excellent ductility in high-entropy alloys with different recrystallization volume fractions

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## Abstract

Concurrent recrystallization and precipitation high entropy alloys recently exhibit superior strength and ductility combination. Here, we successfully obtained the microstructure of micron-scale partially recrystallized and nano-scale heterogeneous precipitates by a facile thermal-mechanical processing. Beyond expectation, three metastable-heterostructure alloys with different recrystallization volume fractions show similar ductility. This stable ductility comes from the similar HDI ductilizing effects. With the *in-situ* strain mapping technique, we firstly verified the existence of hetero-deformation between the discontinuous coarsening-induced lamellar precipitates. And the sources of HDI stress are further investigated to uncover the origin of the stable ductility based on the modified HDI stress calculation modelling. These findings not only provide a facile route to obtain heterogeneous microstructures with stable and excellent mechanical properties but also deepen the comprehension of the multiscale heterogeneous deformation, especially the precipitate-scale hetero-deformation behaviour.

Topic area: High-Entropy Materials and Amorphous Materials (K)

*Keywords: high-entropy alloys, ductility, heterogeneous deformation, discontinuous coarsening*

# TiZrHfNb refractory high-entropy alloys with twinning-induced plasticity

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**Abstract**

The twinning-induced plasticity (TWIP) effect has been widely utilized in austenite steels, β-Ti alloys, and recently developed face-centered-cubic (FCC) high-entropy alloys (HEAs) to simultaneously enhance the tensile strength and ductility. In this study, the TWIP effect through hierarchical {332<113> mechanical twinning has been successfully engineered into the TiZrHfNb refractory HEAs by decreasing temperature and tailoring the content of Nb to destabilize the BCC phase. At cryogenic temperature, the comprehensive hierarchical {332}<113> mechanical twins are activated in $TiZrHfNb_{0.5}$ alloy from micro- to nanoscale and progressively segment the BCC grains into nano-scale islands during deformation, ensuring sustainable strain hardening capability and eventually achieving a substantial 35% uniform tensile elongation. In addition, at 77K, the tensile strength and uniform elongation of $TiZrHfNb_x$ alloys can further be adjusted by a moderate increase of Nb. The results above shed new light on the development of high-performance refractory HEAs with a high and adjustable strength and ductility combination down to the cryogenic temperature.

***Keywords***: *Refractory high-entropy alloys; Cryogenic temperature; Twinning induced plasticity; Hierarchical twins; Tensile properties*

# Technical **Oral Session _ Session 9**

## **Symposium L :** Composite, Coating and Hetero-Materials

**Composite, Coating and Hetero-Materials 9 (L9)** **16:00 -17:25, Nov. 22**

**Chair :** Raj Ladani (RMIT University), Xuexi Zhang (Harbin Institute Of Technology) 202B, 2F

16:00-16:20 **I-L0968** **[Invited] Graphene Reinforced Aluminum Composites Prepared by Drawing**
Mingfang Qian (Harbin Institute Of Technology, China)

16:20-16:40 **I-L0315** **[Invited] Refined Microstructures and Enhanced Strength of in-situ TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si Composites by Selective Laser Melting**
Qi An (Harbin Institute of Technology, China)

16:40-16:55 **O-L0390** **Fatigue-resistant elastocaloric effect in hypoeutectic TiNi58 alloy with heterogeneous microstructure**
Qianglong Liang (Xi'an Jiaotong University, China)

16:55-17:10 **O-L0488** **Wear behaviour of 3d interconnected immiscible Mg-Fe80Cr20 composites synthesized by liquid metal dealloying**
Soo-Hyun Joo (Dankook University, Korea)

17:10-17:25 **O-L0655** **Speeds of Stacked Layers during Cold Roll Bonding**
Hiroshi Utsunomiya (Osaka University, Japan)

# Graphene Reinforced Aluminum Composites Prepared by Drawing

**Mingfang Qian**[1], XueXi Zhang[2], Lin Geng[3]

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## Abstract

Homogeneous dispersion of high-content graphene nano-platelet (GNP) in metals is challenging due to the serious aggregation tendency of graphene. Traditional secondary processing such as extrusion usually has too limited shear strains to reach a desirable GNP dispersion state. Our previous work demonstrated that 1.0 vol% GNP/Al composite was successfully produced via multiple wire-drawing at ambient temperature. However, the fabrication of 5.0 vol% GNP/Al composite was not successful because of the limited cumulative shear strains. Here we described fully dispersed state of 5.0 vol% GNP in Al by hot-drawing at an elevated temperature 400 °C. The evolution of the microstructures and mechanical properties were investigated in relation to the number of drawing passes. The ultra-fine grains with size 372 nm were obtained via dynamic recrystallization after drawing for six passes. In particular, stripping of the GNP into thin layers and their preferential alignment in the wire axis occurred during the shear deformation. As a result, 5.0 vol% GNP/Al composite produced by six-pass drawing possessed improved yield strength and ultimate tensile strength. The results demonstrated the feasibility of dispersing high-content GNP in aluminum alloys via extrusion followed by multi-pass hot drawing techniques.

*Keywords: Graphene nano-platelet (GNP), Aluminum matrix composites (AMCs), Hot extrusion, Multi-pass hot drawing, Mechanical properties.*

# Refined Microstructures and Enhanced Strength of in-situ TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si Composites by Selective Laser Melting

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## Abstract

Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si alloy (Ti-6.5Al-2.5Zr-1Mo-1V) is a near α titanium alloy, which has been widely used in aerospace fields due to its low density, high specific strength, good corrosion resistance and high-temperature durability. To further improve the strength and service temperature of Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si alloy and achieve the near-net-shape manufacturing of complex components, the spherical Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si alloy powder with a particle size of 15~53μm and $TiB_2$ powder with a particle size of 0.5~1μm were used to fabricate in-situ TiBw reinforced Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si composites through low energy ball milling and selective laser melting (SLM). The results show that the TiB whiskers are uniformly distributed in the TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si composites, and the columnar grains with inner acicular α' martensite were formed along the building direction. In addition, the TiB reinforcement effectively refined the size of the matrix grain. The maximum room temperature tensile strength of 2vol.%TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si composite reaches up to 1293.2MPa, but the elongation is only 1%. The tensile strengths of 1vol.%TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si composite and Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si alloy room temperature are 1268.3MPa and 1158.2MPa, respectively. Furthermore, the tensile strengths of 2vol.%TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si, 1vol.%TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si and Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si at 600°C are 651.1MPa, 635.4MPa, and 591.3MPa respectively. Consequently, the TiB whisker has significantly enhanced the strength of Ti alloys. The corresponding strengthening mechanisms include load transfer strengthening, and grain refinement strengthening. However, the plasticity of the composites is decreased. The fracture morphology of the composite at room temperature shows inside porous defects, as well as shallow dimples and tear edges. No traces of TiB whiskers being pulled out, indicating that the TiB is well bonded to the matrix. The high-temperature fracture contains deep dimples indicating a ductile fracture model.

*Keywords: TiBw/Ti-6.5Al-2.5Zr-1Mo-1V-0.5Si composites; selective laser melting; microstructure; mechanical property; strengthening mechanism*

# Fatigue-resistant elastocaloric effect in hypoeutectic $TiNi_{58}$ alloy with heterogeneous microstructure

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**Abstract**

Shape memory alloys with high fatigue life and adiabatic temperature change (ΔTad) are critical for elastocaloric effect in practical refrigeration applications. Here, we report on the discovery of a hypoeutectic TiNi58 alloy by heterogeneous microstructure design to perform ΔTad of 6.1 K after 2 million fatigue loading-unloading cycles. The fatigue-resistant elastocaloric effect is achieved by a highly reversible quasi-linear superelasticity with strength of 2.2GPa and modulus of 44.9GPa. Such stable mechanical behavior is attributed to the unique hypoeutectic heterogeneous microstructure prepared through simple controlled casting and cooling process, as characterized by multi-scale microscopic analysis. The heterogeneous microstructure is consisted of dendrite regions with a Ti2Ni3 precipitates and the surrounding eutectic structure with lath TiNi3 phase. All different intermetallic phases in the heterogeneous microstructure are embedded in the same B2 phase austinite matrix, which is measured with nonuniform Ni content. The cubic structured Ti2Ni3 precipitates with over 5% lattice mismatch strain near interface facilitate inhomogeneous nucleation of martensite and confine the conventional violent stress-induced martensitic transformation together with the measured nonuniform Ni content in B2 phase, leading to controlled continuous strain release in a reversible quasi-linear superelasticity with ultrahigh fatigue stability. The lath intermetallic TiNi3 phase surrounding dendrites regions works as skeletal reinforcement, providing extra mechanical fatigue stability and giving rise to high strength. This work demonstrates the potential of hypoeutectic TiNi58 alloy for long-term elastocaloric service and provide guidance to design new elastocaloric materials with high fatigue resistance in bulk mass through simple controlled casing process.

*Keywords: Heterogeneous Microstructure; Elastocaloric Effect; Fatigue Resistance; Shape Memory Alloy; Superelasticity*

# Wear behaviour of 3d interconnected immiscible Mg-$Fe_{80}Cr_{20}$ composites synthesized by liquid metal dealloying

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## Abstract

For a decade, 3D interconnected heterogeneous composites produced by liquid metal dealloying (LMD) have been studied due to their unique structures and interesting mechanical properties. The abrasive wear behavior of 3D interconnected immiscible Mg and $Fe_{80}Cr_{20}$ composites was systematically studied as a function of the fraction of the hard $Fe_{80}Cr_{20}$ phase and the applied load. Although the composites have a brittle interface due to their immiscible nature, the 3D interconnected structures exhibit outstanding abrasive wear resistance beyond expectations. Highly deformed structures were observed on worn surfaces, and intrinsic wear mechanisms of each phase differed from those of bulk Mg and $Fe_{80}Cr_{20}$ materials. During the wear test, there was a significant increase in the area fraction of the $Fe_{80}Cr_{20}$ phase on the worn surface, and the nano-grained $Fe_{80}Cr_{20}$ layers with a high density of dislocations successfully protected the underlying soft Mg phase. However, when the Mg phase began to be oxidized, the wear mechanism changed to the delamination of the Mg-rich tribo-film. These new findings on improving wear resistance by structural design could serve as a guideline for various applications of heterogeneous 3D architecture materials.

*Keywords: Liquid metal dealloying (LMD), 3D interconnected structure, Metal matrix composites, Heterogeneous materials, Wear.*

# Speeds of Stacked Layers during Cold Roll Bonding

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## Abstract

In roll bonding process to fabricate clad sheets, it is important to clarify the bonding criterion. It was reported that wire brushing on layer surfaces, higher reduction in thickness, etc. are beneficial for bonding. However, the bonding phenomenon has not been understood completely. In this study, changes of layer speeds in the roll bite is focused. Roll bonding experiments of Al/Cu/Al sheets were conducted. An experimental technique was developed to reveal the layer speeds using measured exit speed of an outer layer (forward slip), relative sliding between layers, and layer thickness profile in the roll bite. The Cu layer was found to enter the roll bite always at higher speed than the Al layers. In cases without bonding, the Cu layer flowed faster than the Al layers even after the roll bite. On the other hand, in case of bonding, the Al layers, which entered the roll bite at slower speed than the Cu layer, accelerated remarkably in so that the Al layers caught up with the Cu layers at kinematical bonding point, then the three layers flow for a certain distance at same speed and acceleration, finally ejected together. Real bonding point was identified by the penetrant testing of the specimens obtained by interrupted roll bonding. In cases of bonding, the real bonding point locates somehow downstream of the kinematical bonding point. The bonding strength increased with distance between the bonding point and the minimum gap. Wire brushing shifted the bonding point upstream and make the bonding strength higher.
(250 words)

**Keywords:** clad sheet, relative sliding, surface treatment, bonding strength

# Technical **Oral Session _ Session 9**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 9-1 (N9-1)** **16:00 - 17:30, Nov. 22**

**Chair :** Minkyu Park (Virtual Lab. Inc.) 203, 2F

16:00-16:15 **O-N0581** **Unraveling the electrochemical behavior of Mg based intermetallics: A first-principles study**
Pragyandipta Mishra (Indian Institute Of Technology Madras, India)

16:15-16:30 **O-N1017** **On-the-fly machine learning force field study of liquid-Al/α-Al2O3 interface**
Tao Hu (Shanghai University, China)

16:30-16:45 **O-N0387** **Application of Machine Learning to Optimize Electrodeposition Parameters for Ni-W Alloy Coatings with High Hardness**
Sen Zhai (Hiroshima University, Japan)

16:45-17:00 **O-N0044** **Material-Dlab, A digital research and development platform for metal materials**
Weice Gao (China Iron & Steel Research Institute Group Co., Ltd, China)

17:00-17:15 **O-N0674** **Synthesizability prediction for TiZrNb-Mo heterostructures using positive and unlabeled (PU) learning scheme**
Aamir Malik (KAIST, Korea)

17:15-17:30 **O-N0086** **Research and development of big data application platform for intelligent blast furnace intensive management and control**
Jing Fei (Anshan Iron And Steel Co.,ltd., China)

# Unraveling the electrochemical behavior of Mg based intermetallics: A first-principles study

**Pragyandipta Mishra**[1], Pranav Kumar[2], Lakshman Neelakantan[3], Ilaksh Adlakha[4]

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## Abstract

Magnesium (Mg) alloys have been the center of attention in many engineering industries owing to their excellent properties like low density, high specific strength, and high ductility making them especially useful in the transportation sector as a lightweight material that subsequently reduces energy consumption and $CO_2$ emission. The room temperature ductility and mechanical properties of Mg are usually enhanced by alloying additions. Based on the thermomechanical processing, the presence of critical concentration of alloying element typically leads to the formation of stable binary intermetallic phases with Mg thereby, distinctly altering the microscopic electrochemical properties of the alloy. However, the secondary intermetallic phases in Mg alloys are typically of sub-micron size, thus accurate electrochemical characterization is a challenging issue. Using first-principles calculations, the electrochemical behavior of various Mg intermetallics was comprehensively quantified. Based on the predicted corrosion potential, apart from $Mg_2Ca$ which behaves as an anode to the Mg matrix, the rest of the Mg based intermetallics act as a cathode. The electrochemical polarization behavior of the intermetallics was strongly dependent on surface-mediated properties (surface energy and work function) and chemical bonding characteristics. Finally, the computational framework provides an accurate screening tool that can assist in alloy design and development of coatings.

*Keywords: First-principles; Mg alloys; Mg intermetallics; Electrochemical behavior.*

# On-the-fly machine learning force field study of liquid-Al/α-$Al_2O_3$ interface

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## Abstract

The atomic structure of the liquid Al/α-$Al_2O_3$ interface was investigated using on-the-fly machine learning force field (MLFF) based on first-principles calculations. We found that three different terminal layers of the liquid Al/α-$Al_2O_3${0001} interface exhibited the same characteristics. Liquid Al atoms exhibited a layered phenomenon on the substrate α-$Al_2O_3$ surface, where Al atoms at the interface formed an Al-rich layer and several prenucleation layers. No more than one percent of the first-principles calculations are used in the force field generation process. Therefore, the efficiency of on-the-fly MLFF has been increased by tens of times compared with traditional AIMD. Bayesian error and root mean square error indicate that the error in the simulation is maintained at a small value, suggesting that molecular dynamics simulations with on-the-fly MLFF don't compromise on accuracy. Dynamic analysis techniques such as mean square displacement and vibrational density of states indicated that the Al-rich layer at the interface possesses a quasi-solid nature, while the prenucleation layer was a quasi-liquid. In addition, we simulated a larger system of more than 1000 atoms, which showed that periodic boundary conditions caused size effects that affected the order of the liquid atoms at the interface. The results indicate that on-the-fly MLFF based on first-principles calculations can accelerate simulations of metal/oxide liquid-solid interfaces without sacrificing accuracy, thereby expanding computational time and length scales. Hence, the present study has the potential to generate substantial interest and inspire further research into the utilization of on-the-fly MLFF for simulating various liquid-solid interfaces.

*Keywords: On-the-fly machine learning force field, Ab initio molecular dynamics, Prenucleation, Liquid-solid interfaces.*

# Application of Machine Learning to Optimize Electrodeposition Parameters for Ni-W Alloy Coatings with High Hardness

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## Abstract

The Ni-W alloy coating is widely used due to high hardness and corrosion resistance. The present study is to design a Ni-W electrodeposited coating with high hardness using direct current (DC) electrodeposition and machine learning (ML) methods. In this study, both the collection of data and the preparation of the Ni-W alloy plating were based on sulfate-citrate electrolyte without any additives. Four machine learning models were employed to predict the coating hardness, namely GradientBoosting (GBDT), RandomForest (RF), DecisionTree (DT), and eXtreme Gradient Boosting (XGBoost). Mean Absolute Error (MAE), correlation coefficient ($R^2$) and root mean square error (RMSE) were used to evaluate those models. Pseudo data generated using the random interpolation method were input to the best model to obtain the set of electrodeposition parameters with the highest coating hardness. The results show that XGBoost model achieved the highest performance compared to other models with $R^2$=0.893, MAE=0.0468, and RMSE=0.0633 and the optimal hardness under pseudo data is about 833HV. The feature importance analysis shows that the electrodeposition temperature, current density, and sodium tungstate concentration have the greatest impact on hardness, and increasing these parameters could improve the hardness of the Ni-W coating. These findings provide valuable insights for optimizing the electroplating process and improving the performance of Ni-W coatings.

*Keywords: Ni-W electroplating; machine learning; hardness; XGBoost;*

# Material-Dlab, A digital research and development platform for metal materials

**Weice Gao**[1], Hang Su[2], Heping Liu[2], Yaqing Hou[3,*], Li Yang[3], Xu Sun[3]

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## Abstract

Accelerating the process of new materials from research and development to application has become an urgent need for the manufacturing industry in the Industry 4.0 era. Among them, the development of material genomics engineering technology plays a key role in improving the efficiency of new material development and reducing research and development costs. Our team adheres to the agile research and development concept of "theoretical calculation + big data analysis" and has independently developed the digital development platform for metal materials, Material-Dlab.

This platform is a multi-scale material cloud computing platform that integrates material calculation, process simulation, service simulation, and material big data. Through the development of graphical window scheduling technology and cloud fortress technology, remote, mobile, and queued computing are realized. We have designed and developed a material APP system based on expert experience, encapsulated and deployed more than 600 different calculation scenario APP programs. By developing material data blockchain technology, we have achieved the rights, discovery, and secure sharing of material research and development data.

Currently, the platform has more than 1,200 registered users, with more than 22,000 cumulative computing tasks. It has been applied to the composition design and process optimization of metal materials such as QP steel, hydrogen-resistant steel, and hot-rolled coils, providing a tool system support for improving the efficiency of digital research and development for enterprises.

*Keywords: Multiscale computing, Graphical window scheduling, Materials APP system, Cloud computing, Material big data analysis.*

# Synthesizability prediction for TiZrNb-Mo heterostructures using positive and unlabeled (PU) learning scheme

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## Abstract

Materials design has been greatly aided by computational techniques, where a large number of compositions could be explored to come up with an optimal solution for a particular application, however, the feasibility of computationally generated compositions remained a daunting question. With the advancement in machine learning techniques, computational material design has taken a big leap forward, however, the fundamental question remained about the predicted compositions. In order to build more confidence in machine learning models, researchers have experimentally synthesized the predicted material configurations. Nevertheless, there is an inherent constraint on experimental synthesis, that is, we can only synthesize a limited number of compositions. Therefore, in this study, we developed a computational method to assess the synthesizability of the TiZrNb-Mo heterostructures using a positive and unlabeled (PU) learning scheme. A graph network-based architecture has been used to get predictions for specific modulus values using high entropy alloys data reported in the literature. The predictions were then subject to a PU learning architecture that assigns them a synthesizability score termed high entropy score which ranges between 0 and 1. The configurations having high entropy scores closer to 1 are more likely to be synthesizable. The PU learning scheme thus offers a promising roadmap to explore the synthesizability of predictions received from any machine learning model.

*Keywords: Synthesizability, Heterostructures, Positive and Unlabeled (PU) Learning.*

# Research and development of big data application platform for intelligent blast furnace intensive management and control

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## Abstract

The blast furnaces of Anshan Iron and Steel Group Coporation have completed large-scale and modernization, and a large amount of information technology has been popularized and applied in the process of blast furnaces. This paper takes Anshan Iron and Steel blast furnace group as the research background. Based on big data and industrial internet technology,combing the smelting process mechanism of blast furnace production and using artificial intelligence, cloud analysis and other technologies, the data management platform was used to effectively integrate the data of each process of blast furnace, and design the data asset catalog.Through the establishment of the big data application platform for the intensive control of the blast furnace,the data was carried out multidimensional in-depth mining ,and the intelligent application model of blast furnace was established.The visual intelligent monitoring of the safe production and operation of blast furnace was realized ,as well as the production operation of blast furnace was guided .The overall information and intelligent level of production operation and management of blast furnace has been improved.

*Keywords:intelligent blast furnace;big data;*data asset;artificial intelligence;*visual intelligent monitoring*

# Technical **Oral Session _ Session 9**

## **Symposium N :** Computational Materials and Artificial Intelligence

**Computational Materials and Artificial Intelligence 9-2 (N9-2)** **16:00 - 17:45, Nov. 22**

**Chair :** Hoheok Kim (Korea Institute of Materials Science) 400, 4F

16:00-16:15 **O-N0064** **Data mining of dislocation microstructures by deep learning**
Yuqi Zhang (The Northeastern University, China)

16:15-16:30 **O-N0724** **Development of Ultrahigh Strength Martensitic Steels with Improved Mechanical Properties via Artificial Intelligence-driven Material Design**
YOONJUNG WON (Kookmin University, Korea)

16:30-16:45 **O-N0911** **Studies on damage mechanisms of tungsten and molybdenum under ITER ELM-like heat load**
Lisong Zhang (Dalian University of Technology, China)

16:45-17:00 **O-N0400** **Structural analysis and interstitial site extraction in bcc Fe grain boundaries by persistent homology analysis**
Bohao Zheng (Tohoku University, Japan)

17:00-17:15 **O-N0445** **Gibbs Energy Estimation from Microstructure data by Combining Phase Field Simulation and Machine Learning Technique**
Yusuke Matsuoka (Nagoya University, Japan)

17:15-17:30 **O-N1023** **Simulation Model of Molten Salt Corrosion Using COMSOL**
MaeHyun Cho (Kyung Hee University, Korea)

17:30-17:45 **O-N0431** **Architecture of Materials data infrastructure and Its Application**
Changchang Wang (Central Iron& Steel Research Institute, China)

# Data mining of dislocation microstructures by deep learning

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## Abstract

The microstructure of dislocations can be accessed by the total density of dislocations or the density of geometrically necessary dislocations (GND). The total dislocation density determines the flow strength of a crystal, which, in the case of high dislocation contents, is a quantity very difficult to measure accurately. On the other hand, related to crystal rotations, the GND densities are conveniently measured from electron diffraction experiments or calculated via simulations. Here, a novel and modern approach is proposed to understand the microstructures of dislocations based on deep learning, which estimates the total density of dislocations from a given density of GND distributions. In this method, the convolutional neural networks (ConvNets) are applied to extract the hidden information in the GND distribution maps to understand the microstructures of dislocations. It is demonstrated that the pre-trained ConvNets can be used to predict the distribution of total dislocation density from a small GND density map. Moreover, this technique is further developed to post-process real EBSD images for α-Fe to estimate the average total dislocation density, which corresponds to stress increments from a Taylor hardening assumption that is in good agreement with experimental values. Compared with previous methods involving much effort to track individual dislocations or other quantities, the present machine learning method is quick and convenient to use.

*Keywords: Convolutional neural networks; Dislocation density; Geometrically necessary dislocations; Machine learning.*

# Development of Ultrahigh Strength Martensitic Steels with Improved Mechanical Properties via Artificial Intelligence-driven Material Design

**Yoon-Jung Won**[1], Keun-Won Lee[2], Jae-Bok Seol[3], Ki-Sub Cho[4]

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## Abstract

High Co-Ni secondary hardening martensitic steels are ultrahigh strength materials with significant potential in the defense, aerospace, and automobile industries. Their excellent balance of strength and toughness makes them ideal as advanced structural materials. However, there's a demand for superior performance at a lower production cost. In this study, we used a range of artificial intelligence techniques, including machine learning, inverse design based on a genetic algorithm, and unsupervised learning, to develop an effective methodology for improving the comprehensive mechanical properties of these materials without increasing production costs. A highly accurate machine learning-based regression model was developed for predicting mechanical properties. This model was then used in inverse design, with a genetic algorithm, to explore the material space for desirable mechanical properties. From the resulting candidates, material screening was conducted using unsupervised learning, identifying promising candidates that meet realistic constraints such as fabrication accessibility and production cost. The selected candidates were produced via vacuum induction melting, and their mechanical properties and corresponding microstructures were evaluated. The experimental alloy steels demonstrated promising mechanical properties, notably achieving an ultimate tensile strength of 2.7GPa, surpassing current state-of-the-art ultrahigh strength secondary hardening steels. Furthermore, the expected production cost of these advanced materials is predicted to be lower, achieving the initial goal of the study. These findings clearly demonstrate the effectiveness of AI-driven material design in the development of advanced structural materials.

*Keywords: material design, artificial intelligence, 2.7GPa-grade ultrahigh strength martensitic steels, secondary hardening, genetic algorithm*

# Studies on damage mechanisms of tungsten and molybdenum under ITER ELM-like heat load

**Lisong Zhang**[1], Xianxiu Mei[2,*], Vladimir V Uglov[3]

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## Abstract

The damage mechanisms of plasma-facing materials (PFMs) under edge-localized mode (ELM)-like heat load relevant for fusion reactors, such as ITER, were investigated. The ELM-like heat load experiments were performed on tungsten and molybdenum using compressed plasma flow irradiation. Thermal–mechanical analysis by means of finite element simulations was combined with experimental results to discuss cracking behavior, grain structure evolution and variations of hardness. There were macro-cracks and micro-cracks on tungsten surface and only micro-cracks on molybdenum surface with the main reason of tensile stress generated by rapid cooling. The high ductile-to-brittle transition temperature of tungsten was another necessary condition for the generation of macro-cracks. Moreover, as a result of stress evolution, longitudinal macro-cracks extending perpendicular to the surface experienced transverse transformation within the material. And for micro-cracks, its generation was associated with the embrittlement of the re-solidification, and its width increased with melting depth. When ELM-like heat load was sufficient to melt tungsten and molybdenum, a submicron-sized cellular sub-grain structure was created on their surface due to high temperature gradient of molten layer under the effect of Bénard–Marangoni instability. Rapid directional solidification from the bottom of molten layer to the surface induced the formation of columnar grains. The generated cellular sub-grains increased hardness, and the thermal effect of irradiation and generated columnar grains led to softening. These results help us to understand failure mechanisms in PFMs under extreme operating conditions and are valuable for developing future fusion reactors.

*Keywords: tungsten, molybdenum, ELM-like heat load, compressed plasma flow irradiation, finite element method.*

# Structural analysis and interstitial site extraction in bcc Fe grain boundaries by persistent homology analysis

**Bohao Zheng**[1], Yongjie Zhang[2], Masato Wakeda[3], Goro Miyamoto[4], Tadashi Furuhara[5]

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**Abstract**

The properties of polycrystalline materials are significantly influenced by grain boundaries (GBs). The segregation of solute atoms at GBs plays a major role in the strengthening/embrittling of the material by altering its GB cohesion energy. Atomistic simulations are widely adopted for the investigation of GB segregation, but the information on site location are necessary for such simulations, which remains challenging to obtain for interstitial solutes, especially those in bcc crystals. While the existing method of Voronoi polyhedra analysis is able to locate interstitial sites in the bulk region, its application to GB regions remains disputable as its definition of interstitial sites is based on the atomic structure of perfect crystals.

In this study, we proposed a non-assumptive method to extract the interstitial sites at GBs using persistent homology (PH) analysis. PH analysis is able to identify polyhedra consisting of atoms within an atomistic system, especially ones that deviate from the perfect crystal structure (e.g. at GBs). With the atomistic model of Σ3(111) and Σ5(310) symmetric tilt GBs of bcc Fe, we demonstrated that our new method is able to extract polyhedra of Fe atoms at GBs, of which the centroids correspond with the most stable segregation sites of carbon given by existing DFT calculations.

Furthermore, with the investigation of GB models with different temperatures, we have shown that besides its ability to identify GB interstitial sites, PH analysis can also illustrate the disordering process of GB structures with temperature elevation.

*Keywords: grain boundary structure, interstitials site identification, temperature dependency, persistent homology.*

# Gibbs Energy Estimation from Microstructure data by Combining Phase Field Simulation and Machine Learning Technique

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## Abstract

Since a Gibbs energy plays an important role in the field of materials development, the thermodynamic databases of Gibbs energy have been developed for various systems over the past several decades in the framework of the CALPHAD method.

However, the accuracy of Gibbs energy database is often insufficient for multi-component high-concentration alloys and the alloy systems that are rarely used, because the Gibbs energy has been assessed based on the limited experimental data. In this study, we focus on the fact that a large amount of available microstructural data have not been effectively utilized for Gibbs energy assessment, and propose a new method that combines a phase field (PF) simulation and a machine learning technique for evaluating the Gibbs energy parameters from microstructural data.

In the proposed method, the cost function, meaning the difference between the experimental data and PF simulations, was first defined as a function of the Gibbs energy parameter. Then, the parameters were optimized based on the conventional gradient method, as is often employed in neural network training.

As a case study, we selected the microstructures produced by spinodal decomposition, and numerical tests, called twin experiments, were performed using the calculated microstructures prepared by PF simulation as the synthetic observation data to prove the applicability of this method. The results indicate the proposed method can effectively estimate the Gibbs energy parameter from the microstructural observation data. It is concluded that this method will be applicable to Gibbs energy estimation for the materials with limited experimental data.

*Keywords: Phase field simulation, Gibbs energy, CALPHAD, Automatic differentiation*

# Simulation Model of Molten Salt Corrosion Using COMSOL

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## Abstract

Molten salt reactor(MSR) system is one of the Generation-IV reactor system. MSR system use liquid molten salt as coolant and fuel in normal pressure and high temperature. Therefore, MSR system has superior thermal efficiency and stability. However, molten salt is very highly corrosive material. So, in long-term operation, corrosion is main problem.

In MSR system, fluoride salts are mainly used. FLiNaK molten salt(46.5LiF-11.5NaF-42KF mol%) is representative fluoride salt. In most high temperature environments, materials derive their corrosion resistance from the formation of a protective surface film of an oxide of Cr, Al, or Si. However, in molten fluoride salt these passive oxide films are chemically unstable, and corrosion is driven largely by the thermodynamically driven dissolution of alloying elements into the molten salt environment. There is no resistance film, corrosion occur uniformly by free energy difference of fluoride compounds. Metals that have high negative free energies of fluoride formation are generally more prone to corrosion, that is, they are more likely to form a fluoride compound and dissolve in the salt.In this study, we develop simulation model including these reactions using COMSOL. This model used Tertiary Current Distribution physics in COMSOL. Governing equations are Nernst-Planck equation, Butler-Volmer equation and Nernst equation. According to other studies, Cr corrosion is main corrosion. In model result, when pure salt, current is very low. Also Cr is most corrosive. However HF impurity was there in salt, current is increase. And if flow velocity was increase, Cr corrosion rate was increase too.

*Keywords:MSR,Corrosion, FliNaK, COMSOL*

# Architecture of Materials data infrastructure and Its Application

Changchang Wang[1,2], **Hang Su[3]**, Lina Duan[2]

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## Abstract

Materials data is the basis of materials digital R&D, and the construction of materials data infrastructure is the key to effectively use materials data and accelerate material R&D. At present, there are many materials data infrastructures in the world, and the opening and sharing of data has gradually become an international consensus. In this paper, we analyzed the main challenges and countermeasures faced by the construction of materials data infrastructure, and put forward the general architecture of distributed materials data infrastructure and it key technologies. Based on this architecture, we designed the deployment mode at the edge layer, enterprise layer and industry layer. Besides, we have built some platforms using this architecture, and demonstrated some modules in this paper and showed their functions in the process of material digital R&D.

*Keywords: materials data infrastructure; materials big data; materials digital research and development; distributed database*

# Technical **Oral Session _ Session 9**

## **Symposium O :** Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**Materials for Sustainability (Green Steel, Recycling, and Corrosion) 9 (O9)** 16:00 -17:35, Nov. 22

**Chair :** YOUNG JO KANG ( Dong-A University), Jungshin Kang (Pusan National University) 401, 4F

16:00-16:20 **I-O1143** **[Invited] Upgrading low-grade Cu scrap by the oxidation refining of various impurities**
YOUNG JO KANG (Dong-A University, Korea)

16:20-16:35 **O-O0549** **Efficient deoxidation of off-grade titanium sponge using magnesium metal under an argon and hydrogen mixed gas atmosphere**
Sung-Hun Park (Korea Institute of Geoscience and Mineral Resources, Korea)

16:35-16:50 **O-O0936** **Toward an eco-friendly and cost-effective titanium production process**
Jungshin Kang (Pusan National University, Korea)

16:50-17:05 **O-O0651** **Manufacture of CuTi Alloy via Self-propagation High Temperature Synthesis (SHS) and Thermal Reduction Process from TiO2 Raw Material**
MYUNGSUK KIM (Korea Institute of Industrial Technology, Korea)

17:05-17:20 **O-O1039** **Low-carbon cementitious binders with waste bricks, steel slag and fly ash**
Janitha Migunthanna (Swinburne University of Technology, Australia)

17:20-17:35 **O-O1098** **Can you have your cake and eat it too?'—Simultaneous improvement of strength and corrosion resistance via the microstructure regulation of magnesium alloys**
Mei-Xuan Li (Jilin University, China)

# Upgrading low-grade Cu scrap by the oxidation refining of various impurities

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## Abstract

As the production of electric vehicles abruptly grows, the demand for relevant materials is also increasing. Among them, Cu is not attracting as much attention as major elements of secondary batteries such as Li, Ni, and so forth, but much more amount of Cu will be required for electric vehicles compared to conventional vehicles. On the other hand, the mining and smelting of Cu ore are expected to be limited due to environmental issues. Thus, Cu scrap should be used more actively and intensively.

Low-grade Cu scrap may contain a significant amount of impurity elements, such as Fe and Si. More efficient techniques to remove those elements should be sought. The effect of top oxygen blowing was investigated and the behavior of the competitive removal of Fe and Si was analyzed using their rate constants. Also, in low-grade Cu scrap, there are a few impurity elements, which are difficult to be removed by oxidation refining. For the more effective removal of those elements by oxidation, several flux conditions were compared to find out the optimized refining conditions. While Pb content in molten Cu could be satisfactorily controlled by properly using borax flux, FeO-based flux was appeared to effective in removing Ni below a certain level of content. For deeper refining, it should be further considered that Cu may be excessively lost by continuous oxidation and the secondary phase containing FeO may be suspended in molten Cu.

*Keywords: Cu scrap, oxidation, top-blowing, impurity, flux*

# Efficient deoxidation of off-grade titanium sponge using magnesium metal under an argon and hydrogen mixed gas atmosphere

**Sung-Hun Park**[1,2], Kyung-Hwan Lim[3], Hyunjin Na[4], Tae-Hyuk Lee[1], Ho-Sang Sohn[2], and Jungshin Kang[5,*]

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## Abstract

To enhance the utilization of off-grade titanium (Ti) sponge as a raw material for Ti metal production, an efficient deoxidation process of off-grade Ti sponge was investigated. Based on the results of thermodynamic analysis, magnesium (Mg) metal was used as a reducing agent under an argon (Ar) and hydrogen ($H_2$) mixed gas atmosphere to efficiently decrease the oxygen (O) concentration in the off-grade Ti sponge to below 0.18 mass%, ASTM grade 1 for Ti. In the experiments, Ti hydride ($TiH_2$) powder, produced by hydrogenation of an off-grade Ti sponge, was employed as the feedstock for the deoxidation process. The deoxidation of the $TiH_2$ powder weighing 0.1 – 2.5 kg was performed at 933 K for 12 h using Mg metal in a molten salt mixture of $MgCl_2$ – KCl under an Ar and 10 % $H_2$ mixed gas atmosphere. Under the optimal conditions, the concentration of O decreased from 1.14 mass% to 0.155 mass%, following deoxidation and subsequent acid leaching. These results demonstrate the effectiveness of the proposed deoxidation process in reducing the O concentration in off-grade Ti sponge to less than 0.18 mass%.

*Keywords: recycling, off-grade titanium sponge, titanium hydride, deoxidation, magnesiothermic reduction*

# Toward an eco-friendly and cost-effective titanium production process

**Jungshin Kang[1]**, Sung-Hun Park[2], Kyung-Hwan Lim[3], Hyeong-Jun Jeoung[4], Tae-Hyuk Lee[5]

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## Abstract

The Kroll process is currently used for the production of high-purity titanium (Ti) sponge. However, this process suffers from disadvantages such as high-energy consumption and high processing cost owing to slow production speed. Additionally, a significant amount of low-grade Ti scrap is generated during the Kroll process and subsequent fabrication steps, which cannot be remelted. Therefore, the recycling of Ti scrap is crucial for the establishment of an eco-friendly and cost-effective Ti production process. In this study, we investigate the deoxidation of Ti scrap such as off-grade Ti sponge using magnesium metal in high hydrogen chemical potential. The results demonstrate that the concentration of O in Ti scrap efficiently decreases from 11750 ppm to 1480 ppm. Furthermore, we discuss the development of a method to produce titanium tetrachloride ($TiCl_4$) using Ti scrap and iron chloride waste. This finding highlights the effective utilization of two major wastes in the Ti industry for manufacturing $TiCl_4$, which is utilized in the production of Ti sponge. Considering the growing demand for establishing a sustainable society, the investigation of green and cost-effective Ti production processes becomes increasingly important in the near future.

*Keywords: titanium, titanium scrap, off-grade titanium sponge, titanium recycling, deoxidation*

# Manufacture of CuTi Alloy via Self-propagation High Temperature Synthesis (SHS) and Thermal Reduction Process from $TiO_2$ Raw Material

**Myungsuk Kim**[1], YongKwan Lee[2], Namhun Kwon[3], Sung gue Heo[4], MiHye Lee[5], Jae-jin Sim[6], Seok-Jun Seo[7*]

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## Abstract

Titanium has a high specific strength and excellent corrosion resistance, so it has been mainly used in the aerospace industry and petrochemical equipment industry. However, the current commercial titanium metal manufacturing process has the problems such as the use of harmful gases, high energy consumption compared to production volume and long process cycles. Therefore, it is necessary to develop environmentally friendly technologies to overcome this problem. In this study, the CuTi was produced by synthesizing $Ti_{(O)}$ via self-propagating high-temperature synthesis (SHS) process using $TiO_2$ as the raw material, followed by the thermal reduction process. The SHS is the powder synthesis process in accordance with self-sustaining combustion reaction by ignition under high-pressure atmosphere, and the $Ti_{(O)}$ powder is spontaneously recovered through reduction. Additionally, the thermal reduction is the process for producing titanium metal using a metal reducing agent, and it can be easily reduced to metal without generating harmful gases. Therefore, in order to increase the reaction efficiency, CuTi alloy was prepared by lowering the oxygen content of the $TiO_2$ raw material according to self-propagating high-temperature synthesis and then performing the thermal reduction process.

*Keywords: Titanium, Self-propagation High Temperature Synthesis, Thermal reduction process, CuTi alloy*

# Low-carbon cementitious binders with waste bricks, steel slag and fly ash

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## Abstract

Population increase and economic growth ever escalate the demand for new infrastructure, requiring constant increases in global investment in construction industry to match the increasing demand for buildings and roads. In these constructions, ordinary Portland cement (OPC) is a primary material used. The production of OPC for use in concrete is a major anthropogenic air polluter with its high $CO_2$ emissions and is a major environmental concern for communities worldwide. As a solution, alternative cementitious materials like geopolymer binders are being proposed as a replacement for OPC in concrete. These geopolymer binders are made by combining aluminosilicate materials, such as fly ash and slag, with strong alkali activators like sodium hydroxide and potassium hydroxide. The focus of this research was to examine geopolymer binders as a full replacement for OPC in concrete. To that end, waste clay bricks (WCB) from construction and demolition (C&D) waste were used as an aluminosilicate precursor in these binders, together with industrial by products, namely fly ash from coal power generation and slag from steel production. The work mainly focused on characterisation of materials, development of new cementitious binders and there by production of concrete. Mechanical properties, durability and serviceability characteristics and environmental performance of these materials were comprehensively investigated. These low-carbon cementitious binders can reduce carbon emissions up to 78% and energy consumption up to 85% compared to OPC binders without compromising concrete's mechanical, durability and serviceability performance.

*Keywords: Waste bricks, Slag, Fly ash, Geopolymer, Sustainable materials.*

# ‘Can you have your cake and eat it too?’—Simultaneous improvement of strength and corrosion resistance via the microstructure regulation of magnesium alloys

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## Abstract

Overcoming the inherent strength-corrosion resistance trade-off remains a significant challenge in magnesium (Mg) alloys. The strength of Mg alloys can be improved after artificial aging due to the formation of second phases, however, most of the second phases as the cathode would accelerate the galvanic corrosion of the surrounding Mg matrix. Recent studies by our group have found that the formation of Guinier-Preston (G.P.) zones rather than second phases during aging could enhance the strength of Mg alloys without damaging the corrosion resistance, and even simultaneously improve the corrosion resistance. Therefore, in this presentation, we would discuss in detail the effect of G.P. zones on the corrosion behavior of Mg-Al-Ca dilute alloy. Based on the idea of forming G.P. zones to replace the second phases, we design and develop a novel low-cost, corrosion-resistant, and strong Mg-Al-Mn-Ca-Ce dilute alloy featured with yield strength (YS) of ~194 MPa, ultimate tensile strength (UTS) of ~265 MPa, and corrosion rate (CR) of ~2.2 mm $y^{-1}$. The Ce micro-alloying can significantly improve the corrosion resistance by transforming the Al-Mn phase into Al-Mn-Ce phase, inhibiting detrimental effect of iron (Fe) impurities, and forming a protective Ce-containing surface film. The high strength stems from the combined effect of G.P. zones and fine-grained structure, and the formation of G.P. zones would not deteriorate the corrosion resistance. This presentation could shed light on the design and fabrication of strong and corrosion-resistant dilute Mg alloys to be used in electronic products and automotive bodies.

*Keywords: Magnesium alloy, G.P. Zones, Strength, Corrosion resistance, Microstructure regulation.*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 10

November 23

9:00-10:20

# Technical **Oral Session _ Session 10**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 10-1 (A10-1)** **09:00 – 10:30, Nov. 23**

**Chair :** Nokeun Park (Yeungnam University) Halla Hall A, 3F

09:00-09:15 **O-A0792** **The effect of austenite size and shape on its mechanical stability in advanced high strength steels (AHSS)**
Jie Luo (Monash University, Australia)

09:15-09:30 **O-A0027** **The abnormal carbon redistribution in lath martensite during tempering in Mn-patterned steels**
Dezhen Yang (Beijing Institute of Technology University, China)

09:30-09:45 **O-A0097** **Acceleration of bainitic transformation in a 0.28C – 3.8Mn – 1.5Si steel using chemical heterogeneity**
Ji Hoon Kim (Tohuko University, Japan)

09:45-10:00 **O-A0601** **Enhancing the Mechanical Performance of Resistance Spot Welds of Hot-Stamped Boron-Alloyed Steels by Paint Baking Treatment**
Sunusi Manladan (Dong-Eui University, Korea)

10:00-10:15 **O-A0212** **Development of Al-10% Si coated 1.8 GPa TWB Hot Stamped Parts in Car Body Application**
ChangWook LEE (Hyundai Motor Company, Korea)

10:15-10:30 **O-A0593** **Microstructural evolution during tempering in an ultra-high strength steel strengthened by coexisting nanoprecipitates**
Haofei Zhu (Beijing Institute of Technology, China)

# The effect of austenite size and shape on its mechanical stability in advanced high strength steels (AHSS)

**Jie Luo**[1], Artem Arlazarov[2], Christopher Hutchinson[1]

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**Abstract**

Steel researchers continually strive to develop AHSS with applications for the automotive industry. A key design consideration in AHSS is leveraging the transformation-induced plasticity (TRIP) effect from the deformation-induced austenite-to-martensite transformation.

Despite recognizing the importance of understanding the TRIP effect, unresolved questions persist regarding the mechanical stability of austenite due to the complexities involved in deconvoluting different factors affecting the stability. The stability of austenite depends on the chemical composition, grain size, and morphology of the grains and also the constraints from the surrounding phases. Few studies dedicated to deconvoluting these factors exist. Moreover, the variation between local and average measurements of strain-induced martensite can be significant due to stress/strain partitioning, and an understanding must be achieved at both the global and local scale of the microstructure.

This talk presents statistical analyses on the influence of austenite grain size and shape on its mechanical stability against local strain. The studied Fe-0.1C-5Mn (wt. %) steels were prepared under the conditions where the composition of austenite grains was constant, but the grain size or shape varied. With coupled microscopic-digital image correlation (micro-DIC) and quasi in-situ electron backscattered diffraction (EBSD) testing, the findings statistically support previous reports of an intrinsic size effect (i.e. smaller is more stable) for globular-shaped austenite in a ferritic matrix. More interestingly, the previously reported shape effect is shown to be essentially a size effect when considered in terms of the local strain experienced by each austenite grain before the transformation.

*Keywords: austenite stability, medium-Mn steels, deformation-induced martensitic transformation, strain partitioning, digital image correlation*

# The abnormal carbon redistribution in lath martensite during tempering in Mn-patterned steels

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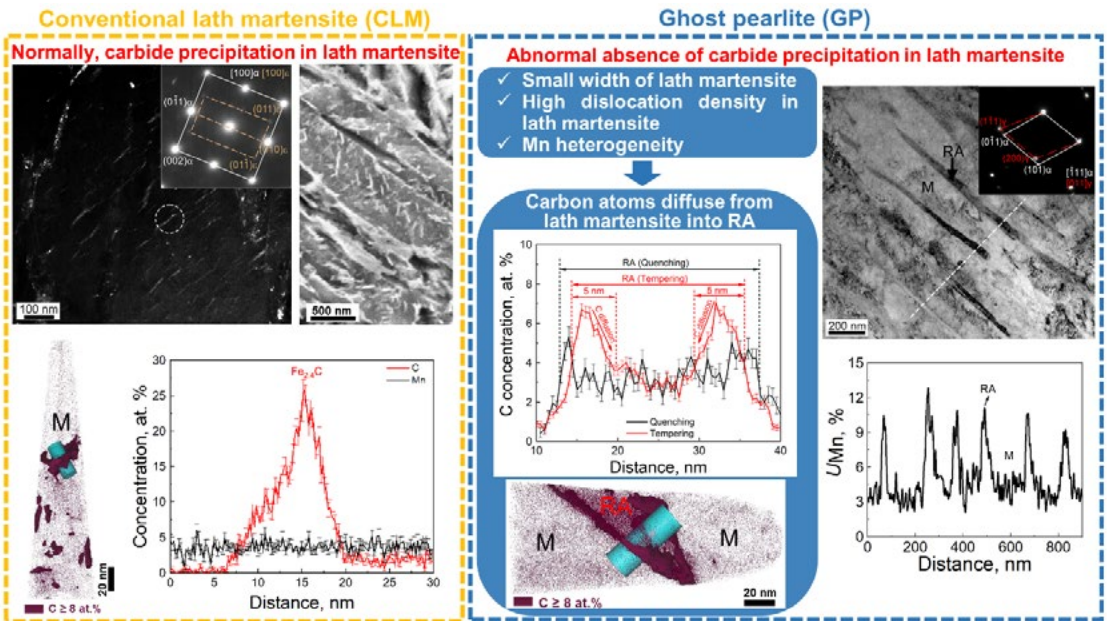
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## Abstract

Martensite tempering is a critical step to achieve high strength with decent ductility. It is well-known that, during tempering, the carbon is sequentially arranged as segregation, transition carbide and cementite. Abnormally, the present study shows the absence of carbide precipitation during tempering in a Si-free pearlite-based quenched and tempered steel. After fast heating and short austenitization from Mn-partitioned pearlite, the high-temperature austenite, which has formed from Mn-depleted ferrite and Mn-enriched cementite, is chemically Mn-patterned, which in turn forms a ghost pearlite composed of alternative Mn-depleted lath martensite and Mn-enriched film retained austenite (RA). During tempering up to 300 °C, the carbide formation is abnormally prevented in martensitic laths. Instead, the carbon atoms diffuse from lath martensite to its neighboring Mn-enriched film RA, which is assisted by a high dislocation density and a small width of lath martensite. Additionally, this RA can promote the carbon diffusion in the interior due to its gradient Mn distribution. All the above inhibit carbide precipitation.

*Keywords: Martensite; retained austenite; partitioning; tempering; carbide precipitation.*



# Acceleration of bainitic transformation in a 0.28C – 3.8Mn – 1.5Si steel using chemical heterogeneity

**Ji Hoon Kim[1]**, Guiyoung Gu[2], Seok-Hwan Hong[3], Changjae Yu[4], Alireza Zargaran[5], Eun-Young Kim[6], Minseo Koo[7], Jae Sang Lee[8], Dong-Woo Suh[9]

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## Abstract

The amount of Mn addition in advanced high-strength steel is increasing to secure sufficient hardenability and stabilize austenite. However, one of the drawbacks of Mn-containing steel is that bainitic microstructure, which effectively improves mechanical properties, is difficult to fully utilize due to its lengthy austempering time.
In this study, one of the ways to accelerate bainitic transformation in Mn-containing steel was suggested. Unlike previous strategies that increased the number of preferential nucleation sites for bainitic transformation by introducing athermal martensite, grain refinement, and deformation, we introduced Mn chemical heterogeneity by applying intercritical annealing prior to full austenitization (i.e., two-step annealing). In the two-step annealed (TSA) steel, bainitic ferrite was rapidly nucleated at Mn-depleted austenite due to a higher driving force, and the bainitic ferrite acted as a nucleation site for subsequent bainitic transformation in Mn-enriched austenite. As a result, the time required to obtain a similar fraction of bainitic ferrite was halved in TSA steel compared to conventionally annealed (CA) steel. Additionally, TSA steel was more advantageous in increasing the fraction of retained austenite ($V_\gamma$) than CA steel. In contrast to CA steel, which stabilizes austenite by C partitioning only during austempering, austenite in TSA steel was not only stabilized by C partitioning during austempering, but also by pre-partitioned Mn during intercritical annealing. With the help of stable retained austenite, TSA steel exhibited superior tensile strength × total elongation balance (TS × TE) compared to the CA steel.

*Keywords: Bainitic transformation, high-strength steel, chemical heterogeneity*

# Enhancing the Mechanical Performance of Resistance Spot Welds of Hot-Stamped Boron-Alloyed Steels by Paint Baking Treatment

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## Abstract

The resistance spot welding (RSW) of ultra-high strength steels is associated with problems such as high susceptibility to interfacial failure and the formation of *halo ring* (a local decarburized and softened region) at the fusion boundary, which affects the failure behavior and energy absorption of the joints. Eliminating the *halo ring* has become a subject of particular interest in RSW of advanced high strength and ultra-high strength steels. Since the paint baking (PB) is an integral part of the car body manufacturing process, it is of paramount importance to investigate the possibility of eliminating the *halo ring* and improving the mechanical performance of the joints using the PB thermal cycle. This would eliminate the need for taking extra steps that would increase the production cost and time. In this study, the resistance spot weldability of two different grades of ultra-high strength B-alloyed steels has been investigated: 1.8 GPa and a novel 2.0 GPa hot-stamped steels. The effect of PB on the microstructure, *halo ring* severity, and mechanical behavior of the joints under different loading conditions has been investigated. The PB process resulted in elements redistribution, elimination/drastic reduction of the *halo ring* severity, and low-temperature tempering of martensite in different regions of the joints. Consequently, the PB joints exhibited better mechanical performance, with superior energy absorption compared to the as-welded joints.

*Keywords: Resistance spot welding, hot-stamping, halo ring, paint baking, fracture behaviour.*

**Acknowledgments**: This work was supported by the Competency Development Program for Industry Specialists, and the Technology Innovation Program (Alchemist Project, 20012196, Al based supercritical materials discovery) funded by the Ministry of Trade, Industry & Energy, Korea.

# Development of Al-10% Si coated 1.8 GPa TWB Hot Stamped Parts in Car Body Application

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**Abstract**

The hot stamping technology has been steadily developed because of providing both excellent formability and high strength. With the development of TWB hot stamping technology, it is now possible to freely apply the required strength and thickness in the right place. In this study, the microstructure and collision performance according to the strength combination of TWB hot stamped parts was evaluated. Through the dilatometry analysis, the hot stamping heat treatment temperatures of 22MnB5 steel and 30MnB5 steel were set at 950 ˚C and 870 ˚C. The 5MnB8 steel was composed of Bainite + Martensite when heat-treated at 950 ˚C and provided strength of 980 MPa grade. When heat-treated at 870 ˚C, it was composed of Ferrite + Bainite + Martensite and provided strength of 780 MPa grade. The simulation of the rear impact test showed the best performance of the 30MnB5-5MnB8 TWB combination because the 5MnB8 part of the 780 MPa grade absorbed enough energy and the 30MnB5 part of the 1.8 GPa grade fully served as an anti-intrusion.

*Keyword: Hot stamping, Al-10%Si coating, Tailor Welded Blank (TWB), 30MnB5*

# Microstructural evolution during tempering in an ultra-high strength steel strengthened by coexisting nanoprecipitates

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## Abstract

In answer to reduce raw materials cost, several low-Co element ultra-high strength steels have been developed. However, due to the harmful effect of Co reduction on the kinetics of secondary phase precipitation, the toughness of these steels is usually not comparable with the high-Co ones. This work develops a low-Co steel that is synergistically strengthened by $M_2C$ carbide and NiAl intermetallic compound, in which NiAl boots the nucleation of $M_2C$. It exhibits yield strength of 1883 MPa and impact toughness of 28 J, showing the comparable strength and toughness with Aermet310 steel. The microstructural evolution during tempering and precipitation strengthening mechanisms are analyzed based on transmission electron microscopy. Under peak aging conditions, both the needle-like $M_2C$ carbide and spherical NiAl intermetallic compounds are coherent with the matrix. The contributions of $M_2C$ and NiAl precipitates to strengthening are 856 MPa and 425 MPa, respectively, which are evaluated by Orowan looping and precipitates shearing. As the precipitation proceeds, the $M_2C$ gradually coarsens and loses coherent with matrix, while the NiAl precipitates are still coherent with matrix. Meanwhile, the film reverted austenite form between the martensite laths, contributing to the improvement of toughness.

*Keywords: ultra-high strength steels; toughness; precipitation strengthen; reverted austenite.*

# Technical **Oral Session _ Session 10**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 10-2 (A10-2)** **09:00 – 10:30, Nov. 23**

**Chair :** Seok Su Sohn (Korea University) 303B, 3F

09:00-09:15 **O-A0364** **In-situ ECCI of Dislocation Structure Evolution during Plastic Deformation in Lath Martensite of Low-Carbon-Steel**
Shuang Gong (The University of Tokyo, Japan)

09:15-09:30 **O-A0613** **Effect of cooling rate on the improvement of tensile properties in a Fe-Mn-Si-C-based multi-phase TRIP steels**
Chang-Gon Jeong (Pohang University of Science and Technology, Korea)

09:30-09:45 **O-A0421** **Intercritical Austenitizing, Room Temperature Quenching, Tempering and Partitioning (IA-Q-T&P): Enhancing Yield Strength and Preventing Plastic Instability**
Juhua Liang (Hefei Institutes of Physical Science, Chinese Academy of Sciences, China)

09:45-10:00 **O-A0472** **Role of cementite during austenitization in auto-tempered 0.15C-5Mn martensitic steel**
Jungwoong Kim (Pohang University of Science and Technology, Korea)

10:00-10:15 **O-A0035** **Restraining plastic instability of intercritically annealed 7Mn medium-Mn steel via pre-water quenching**
Mei ZHANG (Shanghai University, China)

10:15-10:30 **O-A0972** **Effect of strain rate on tensile behavior of Fe-Mn-Al-Cr-C steel**
Dong Hyuk KIM (Pohang University of Science and Technology, Korea)

# In-situ ECCI of Dislocation Structure Evolution during Plastic Deformation in Lath Martensite of Low-Carbon-Steel

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## Abstract

Lath martensitic steels are widely used iron-based alloys with outstanding mechanical properties. However, despite its high yield strength, it shows very weak ductility. So, it is necessary to understand the microscopic mechanism of plastic deformation in lath martensite. It has been clarified that lath martensite exhibits significant anisotropy in local deformation behaviour. The anisotropy has been discussed in relation to the fact that the lath habit plane is approximately parallel to {110} and the active slip direction <111> in bcc, which can divide slip systems into in-lath-plane and out-of-lath-plane slip systems, while the underlying mechanisms are still under debate.

In this present study, in-situ tensile Electron Channeling Contrast Imaging (ECCI) observations were performed to reveal the evolution of dislocation structure in the blocks with different combinations of potentially active slip systems i.e., in-lath-plane and out-of-lath-plane slip systems.

The motion of dislocations and the microscopic strain revealed that the slip systems with high Schmid factors are primarily activated and contribute to plastic deformation. Macroscopic yielding occurs when the increasing applied stress causes dislocations to transmit their barriers, such as high-dislocation-density walls, within the grains. Even though the order of the active slip systems is determined only by their Schmid factors, the amount of local plastic deformation is highly dependent on the type of active slip system, that is, the activation of the in-lath-plane slip system will result in much greater plastic deformation than that in the case where only out-of-lath-plane slip systems are activated.

*Keywords: Lath martensite, Plastic deformation, Dislocation, In-situ ECCI*

# Effect of cooling rate on the improvement of tensile properties in a Fe-Mn-Si-C-based multi-phase TRIP steels

**Chang-Gon Jeong**[1], T.T.T. Trang[2], Youngyun Woo[3], Eun Yoo Yoon[4], Young-Seon Lee[5], Yoon-Uk Heo[6*]

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## Abstract

The commercial fastener has been produced through two different types of process; quenching&tempering or non-quenching&tempering. There are several additional processes in the quenching&tempering system, e.g. spheroidizing, and straightening, and it possibly leads to a considerable cost in production. Therefore, the non-quenching&tempering system has drawn attention in the cold-forging process even though many challenges remain; low tensile strength or high yield ratio. The multi-phase TRIP steel has been studied to apply the non-quenching&tempering process due to its attractive mechanical properties such as low yield strength and high work hardening rate. The classical two-step heat treatment (intercritical annealing and bainitic isothermal treatment) was adapted to obtain the required mechanical properties. However, there is a lack of understanding of the cooling effect on the microstructural evolution and mechanical properties. In addition, the explanation of role of constituent phase, except for retained austenite, is insufficient to analyze the behavior of deformation-induced martensitic transformation (DIMT).

This study firstly investigated the cooling rate-dependent microstructural evolution. Then, tensile properties in different microstructures were evaluated. The improvement of tensile properties was achieved without trade-off of elongation as increase the cooling rate. In order to understand clearly work hardening behavior, the in-situ experiment characterized the kinetics of DIMT and its result was compared with that of XRD. The effect of the microstructural evolution on the mechanical properties and the kinetics of DIMT depending on the cooling rate is further discussed.

*Keywords: Phase Transformation, Multi-phase TRIP Steel, Austenite Stability, In-situ Characterization, Kinetics of Strain-Induced Martensitic Transformation*

# Intercritical Austenitizing, Room Temperature Quenching, Tempering and Partitioning (IA-Q-T&P): Enhancing Yield Strength and Preventing Plastic Instability

**Juhua Liang**[1], Xingfu Wang[2], Zimu Shi[3], Fusheng Han[4], Jiangtao Liang[5], Zhengzhi Zhao[6]

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## Abstract

In the research on third-generation advanced high-strength steel, particularly in automotive applications, short-time and low-temperature treatments are commonly used to achieve ultra-fine microstructure and high strength, owing to the high-speed continuous annealing production characteristics of thin strips. However, for thick-sized special steels, prolonged heating is necessary, making quenching and tempering (Q-T) and austenite reverse transformation annealing (ART) more suitable. This study presents a novel heat treatment process called Intercritical Austenitizing, room temperature Quenching, Tempering and Partitioning (IA-Q-T&P), applied to a 4wt. % manganese alloy steel. The process eliminates the need for precise temperature control during quenching and partitioning (Q-P), requiring only room temperature quenching. It effectively mitigates plastic instability phenomena, such as dynamic strain aging (DSA) and Portevin-Le Chatelier (PLC) effects, which are typically observed in traditional ultrafine-grained medium manganese steel, as confirmed by the engineering stress-strain curve. The IA-Q-T&P process generates a multi-phase microstructure consisting of ferrite, tempered martensite, retained austenite, and carbide precipitation. It demonstrates a remarkable enhancement in yield strength, with values increasing from 698 MPa to 971 MPa, while also attaining higher tensile strength of 1465 MPa and a comparable total elongation of 22.9% compared to the ART process.

*Keywords: yield strength, intercritical austenitizing, quenching and partitioning, tempered martensite*

# Role of cementite during austenitization in auto-tempered 0.15C-5Mn martensitic steel

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**Abstract**

Effects of cementite and auto-tempering on the microstructure and mechanical properties of 0.15C-5Mn (wt.%) martensitic steels were investigated by adjusting the austenitizing temperature and cooling rate. The tensile strength and elongation of the material decreased with an increase in austenitizing temperature in both air cooled and water quenched conditions, and air cooled samples showed lower strength and higher elongation than water quenched ones. Specifically, in the case of air cooling, the sample austenitized at 800 °C exhibited better strength (200 MPa) and elongation (4 %) compared to the sample austenitized at 1000°C. The sample austenitized at low temperature had a higher retained austenite volume fraction. Due to low Mn diffusivity, cementite formed during coiling simulation was changed to retained austenite after austenitizing at low temperatures, which improved tensile properties through the TRIP effect. During air cooling, auto-tempering occurred, which resulted in a decrease in strength and an increase in elongation by martensitic softening. Furthermore, auto-tempering improved the stability of the retained austenite as the carbon diffused into it. As a result, there was a relatively large elongation difference between air cooled and water quenched samples at 800 °C compared to samples above 900 °C.

*Keywords: martensitic steel; retained austenite; auto-tempering; Mn partitioning; cementite*

# Restraining plastic instability of intercritically annealed 7Mn medium-Mn steel via pre-water quenching

**Mei Zhang[1]**, Qiongying Cen[2], Jie Zhang[1], Han Dong[1]

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## Abstract

This study focuses on restraining the plastic instability and maintaining excellent mechanical properties of 7Mn medium-Mn steel (MMnS) via the inclusion of a pre-water quenching (WQ) step before the traditional intercritical annealing (IA) treatment (at 630 °C for 1, 2, 4 and 8 h). The cold-rolling alloy was austenitized at 850 °C for 0.5 h and then water-quenched to room temperature in advance to adjust the original and final microstructures. The pre-WQ step caused the final ferrite and austenite dual-phase morphology to change from nano-equiaxed to nano-lamellar + equiaxed. The sample after traditional IA at 630 °C for 1 h exhibited excellent comprehensive mechanical properties, with a product of ultimate tensile strength and total elongation (UTS·TEL) of 48.9 GPa·%; however, the yield point elongation (YPE) indicating typical plastic instability was as high as 17%. In contrast, the sample after WQ+IA at 630 °C for 4 h showed a similar UTS·TEL of 42.2 GPa·%, but the plastic instability phenomena, including the formation of Lüders bands (related to the YPE) and PLC bands, were greatly restrained. This was due to the low degree of recrystallization, mixed morphology of the final microstructure, high original dislocation density in ferrite, and fine grain size resulting from this treatment. Additionally, the substitution of TEL with meaningful favorable plasticity (MFP) (TEL-YPE) allowed a more accurate assessment of the comprehensive properties of MMnS. The as-prepared Lüders-band-free MMnS, with outstanding comprehensive mechanical properties, is of great significance owing to its extensive application potential in the automotive industry.

*Keywords: Medium manganese steel, Microstructure control, Restraining plastic instability, Deformation mechanism, heat treatment combination.*

# Effect of strain rate on tensile behaviour of Fe-Mn-Al-Cr-C steel

**Dong Hyuk Kim[1a]**, Joe Jun[2], Sung-Joon Kim[1b]

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## Abstract

The weight reduction of structural materials plays a crucial role in environmental protection. To achieve this, Fe-Mn-Al-C duplex steel was developed by incorporating aluminum (Al), while chromium (Cr) was added to enhance corrosion resistance. It is imperative for structural materials to exhibit excellent mechanical properties in both quasi-static and dynamic deformation modes, ensuring the safety.

The comprehension of the quasi-static and dynamic tensile behavior of Fe-Mn-Al-C-Cr is of paramount importance, considering the requirements for mechanical properties in structural materials. We prepared Fe-15Mn-6Al-5Cr-0.2C for investigating the tensile behavior with different strain rate. Electron Backscatter Diffraction (EBSD) and Scanning Electron Microscope with Energy Dispersive Spectroscopy (SEM-EDS) observations were conducted to analyze the microstructure. Tensile tests were performed at various strain rates to observe changes in the mechanical properties of the material. Furthermore, the fracture surface and microstructure of the tensile tested specimens were examined to understand variations influenced by the strain rate.

*Keywords: Strain rate, high Mn steel, tensile test, mechanical properties*

# Technical **Oral Session _ Session 10**

## **Symposium B :** Advanced Processing of Materials

**Advanced Processing of Materials 10 (B10)** **09:00 - 10:00, Nov. 23**

**Chair :** Soon Jik Hong (Kongju National University), Matthias Weiss (Deakin University) **301, 3F**

09:00-09:30 **K-B** **[Keynote]**
Matthias Weiss (Deakin University, Australia)

09:30-10:00 **K-B1174** **[Keynote] Development of high-performance materials through advanced powder manufacturing processes**
Soon Jik Hong (Kongju National University, Korea)

# Development of high-performance materials through advanced powder manufacturing processes

**Soon-Jik Hong**

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**Abstract**

The development of advanced materials processing such as casting, powder metallurgy (PM), and additive manufacturing (AM) has played an important role in manufacturing new metal materials. Powder metallurgy (PM) is a widely used metal-forming technology to fabricate dense and precise components. Different powder and component forming routes can be adapted to yield a product with properties tailored for specific applications or industries. Notably, powder metallurgy explores a range of materials and techniques that are being widely used for different application areas. The controlled processing of these powders determines the material's final mechanical and tribological properties. Various fabrication routes are employed to customize these powders, including gas atomization, water atomization, and mechanical alloying. These processes offer advantages such as grain refinement and the supersaturation of alloying elements, improving mechanical properties. Advanced consolidation processes are also being explored to create layered structures and composites with superior properties. This presentation aims to provide a comprehensive review of the state-of-the-art methodologies in developing metal powders through PM approaches, highlighting the main concepts and recent advancements in fabrication, especially in gas atomization, water atomization, and mechanical alloying. We will discuss their mechanical, tribological, and thermal properties for structural and functional applications, innovations that redefine conventional PM processes, and the role of different consolidation processes in fabricating layered structures and composite materials.

*Keywords: Powder metallurgy, Additive manufacturing, Microstructure, Mechanical properties, Tribology.*

# Technical **Oral Session _ Session 10**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 10 (D10)** **09:00 -10:05, Nov. 23**

**Chair :** Xiaodong Peng (Chongqing University) Samda Hall A, 3F
Byeong-Chan Suh (Korea Institute of Materials Science)

09:00-09:30 **K-D0357** **[Keynote] Kink strengthening of layer-structured Mg alloys**
Eiji Abe (University of Tokyo, Japan)

09:30-09:50 **I-D0343** **[Invited] Kink Strengthening of Mille-Feuille-Structured Mg-Zn-Y Alloys with α-Mg Single Phase**
Yoshihito Kawamura (Kumamoto University, Japan)

09:50-10:05 **O-D0185** **Ball indentation behavior in magnesium single crystals**
Hiromoto Kitahara (Kumamoto University, Japan)

# Kink strengthening of layer-structured Mg alloys

Eiji Abe

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## Abstract

Dilute Mg alloys containing a few atomic percent of transition-metal and rare-earth element have attracted increasing attentions because of their excellent mechanical properties. The remarkable microstructural feature common for all of these Mg alloys is formation of a novel type of long-period stacking/order (LPSO) structures, which reveal a remarkable strength through the warm-extrusion process. During the process the LPSO crystals are deformed not by simple dislocation migrations but of kink-type that is the direct relevance to realize excellent properties of the alloys. From the extensive studies of the LPSO-structured Mg alloys for more than a decade, it has become apparent that the kink regions indeed play a critical role for effective strain storage of the alloys, but its detailed mechanism is not fully understood yet.

In order to deepen our understanding of the veiled work-hardening mechanism related to kink, we have studied the “Kink strengthening phenomenon”, which could be a universal strengthen principle for the design of novel light alloys. In the meantime, the LPSO structure can be generally viewed as “Mille-feuille structure (MFS)”, in the sense that they are constructed by alternate stacking of microscopic hard- and soft-layer. Our studies have confirmed that the MFS Mg alloys indeed reveal the kink strengthening, whose effect seems to be more prominent than LPSO Mg alloys. Therefore, solving the critical condition and universality on the kink-strengthening phenomenon will certainly lead to a further development of lightweight structural materials, including novel Al and Ti alloys in the future.

*Keywords: magnesium alloys, long-period stacking/order (LPSO), microstructure analysis, scanning transmission electron microscopy (STEM), computations and modelling.*

# Kink Strengthening of Mille-Feuille-Structured Mg-Zn-Y Alloys with α-Mg Single Phase

**Yoshihito Kawamura**[1]

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**Abstract**

Kink strengthening, discovered in the LPSO phase, is considered a new strengthening method for materials. Kink strengthening is also found to occur in mille-feuille structured materials with a stacked structure of hard and soft layers. We have successfully produced a mille-feuille structured Mg-Zn-Y alloys with an alpha-Mg phase, which have cluster arranged nanoplates (CANaPs) consisted of cluster arranged layer (CAL) and Mg layer. The mille-feuille structure (MFS), including the thickness and dispersion of CANaPs, could be controlled in the range of 1.2-7.0 nm and 0-0.055 $nm^{-1}$, respectively, by both aging conditions and alloy composition. The MFS structure was found to recrystallize more easily than the LPSO structure. The Mg-0.4Zn-1.0Y (at%) alloy with a CANaP thickness of 1.9 nm and a CANaP dispersion of 0.053 $nm^{-1}$ was able to suppress dynamic recrystallization (DRX) during hot extrusion at an extrusion temperature of 598 K, an extrusion ram speed of 1.5 mm/s and an extrusion ratio of 6 or less. The tensile yield strength and elongation of the Mg-0.4Zn-1.0Y alloy before extrusion were 115 MPa and 8.3%, respectively. The extruded MFS Mg-0.4Zn-1.0Y alloy without DRX exhibited a high yield strength of 418 MPa and a moderate elongation of 5.8 %. Kinking was observed in the non-DRXed MFS alloy. The kink disappeared in DRXed grains of the MFS alloy extruded at an extrusion ratio of 7.5 or higher. The grain size was reduced by DRX from 35.5 to 1.5 micrometer. Yield strength decreased and elongation increased with the progress of dynamic recrystallization.

*Keywords: LPSO, MFS, Kink Strengthening, Extrusion, Recrystallization.*

# Ball indentation behavior in magnesium single crystals

**Hiromoto Kitahara**[1], Ryu Ohkubo[2], Shinji Ando[3]

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## Abstract

We reported on crystal orientation dependence of ball indentation behavior on low-index planes in pure magnesium single crystals; indentation morphology showed circular on (0001) and elliptic on both (10-10) and (11-20) planes. In this study, an instrumented microhardness tester was used to obtain load-penetration curves to quantitatively evaluate the indentation behavior. Also, other crystal planes between low-index planes were systematically investigated. With increasing tilt angles between (0001) and indented planes, the aspect ratio of indentations increased and the indentation morphology became more elliptical. Basal slips and {10-12} twins were observed around all indentations. Different types of {10-12} twins, twin variant, were observed; two twin variants were observed when the indented planes were tilted more than 45 degrees from (0001) and more than 15 degrees from (10-10). Also, with increasing tilt angle from (0001), the slope of the loading curves decreased and the indentation depth increased. Using the systematic indentation data obtained in this study, unknown crystal orientations of magnesium single crystals are identified only by the ball indentation test without X-rays. The accuracy of crystal orientation determination was within 15 degrees in this study. The indentation method for the determination of crystal orientations could be used for the life assessment of huge and/or immobile structural parts under fatigue conditions resulting in crystal rotations, set in environments where X-rays are not allowed to use.

*Keywords: Load-Penetration curve, {10-12} twin, Basal slip, pyramidal slip,*

# Technical **Oral Session _ Session 10**

## **Symposium E :** Additive Manufacturing

### Additive Manufacturing 10-1 (E10-1) — 09:00 - 10:25, Nov. 23

**Chair :** Tsuyoshi MAYAMA (Kumamoto University)
Feng He (Northwestern Polytechnical University)
Halla Hall B, 3F

09:00-09:30 **K-E1162** **[Keynote] Constitutive Model and Finite Element Simulation of Additive Manufacturing Metallic Materials**
Hyoung Seop Kim (Pohang University of Science and Technology, Korea)

09:30-09:50 **I-E0235** **[Invited] Potential microstructural descriptors of additive-manufactured 316L stainless steel**
Yoshitaka ADACHI (Nagoya University, Japan)

09:50-10:10 **I-E1178** **[Invited] Melt pool flow induced uniform dispersion of reinforcing particles in additively manufactured metallic composites**
Li Zan (Shanghai Jiao Tong University, China)

10:10-10:25 **O-E0124** **Effects of Laser Powder Bed Fusion (LPBF) process parameters on Ti6246 microstructure and mechanical properties.**
Prince Cobbinah (The University of Tokyo, Japan)

# Constitutive Model and Finite Element Simulation of Additive Manufacturing Metallic Materials

**Hyoung Seop Kim**[1], JiHye Kwon[2]

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## Abstract

Engineering metallic materials are an essential class of materials for a variety of industrial applications due to their competitive mechanical properties, especially strength and ductility. Metallic materials with excellent mechanical properties are highly sought-after as engineering materials for various applications considering safety, environmental, and economic requirements. Thus, the development of high-performance alloys with high strength and high ductility is an unfading research topic for material scientists. The strength enhancement in metallic materials by conventional strengthening mechanisms always leads to a reduction in ductility, which is often referred to as strength-ductility trade-off. In recent decades, novel approaches to enhance strength-ductility synergy through heterogeneous microstructures, such as gradient, harmonic, lamellar, bimodal, hierarchical nanostructures, etc., have been proven to be effective in overcoming strength-ductility trade-off. In this presentation, a constitutive description of MAM materials was developed and an attempt to maximize the back stress strengthening effect by tailoring the microstructures of multi-gradient heterostructures that were fabricated using metal additive manufacturing. Compared to conventional heterogeneous materials that consist of one or two gradient structures, the multi-gradient heterostructure fabricated using the proposed method comprises four regions with different microstructural features and mechanical properties. The mechanism behind the mechanical properties of the multi-gradient heterostructured material is investigated, with a focus on the multi-gradient microstructure and the back stress strengthening effect.

*Keywords: Metal additive manufacturing, Constitutive model, Cellular structure; Dislocation density, Finite element analysis*

# Potential microstructural descriptors of additive-manufactured 316L stainless steel

**Yoshitaka Adachi[1], Fei Sun[1], Yuichiro Koizumi[2], and Takayoshi Nakano[2]**

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[2] Osaka University, Division of Materials Science and Engineering, , Suita, 565-0871, Japan



## Abstract

Additive manufacturing (AM) allows a variety of microstructures to be formed, which often results in unusual material properties. Microstructure produced by AM is very anisotropic compared with one by conventional casting. Therefore, very careful microstructural characterisation is really required. Furthermore, microstructure is usually observed in two-dimension (2D), which is sometimes not adequate to fully assess complicated microstructures produced by AM method. Therefore, three-dimensional (3D) observation is sometimes performed by serial sectioning or tomography method. Those methods are, however, time-consuming and require special devices in common.

To understand extraordinary properties of AM material, microstructures should be fully quantified in 2D and hopefully in 3D. Scale-bridging analysis using various characterisation methods and 3D microstructural reconstruction contributes to quantitatively analyse microstructures in wide scale range. Machine learning is very useful to correlate properties with microstructure characteristics such as grain size, volume fraction and so on. Hierarchical microstructure features obtained are to be input into machine learning to estimate an output such as a property.

This study will focus on an unknown microstructural feature of AM-316L stainless steel produced by a laser bed fusion method that was managed by Osaka University. High-resolution HAADF-STEM unveils an unknown microstructural feature, and also a new generative adversarial network (GAN) realises to demonstrate a reliable 3D microstructure which was reconstructed from only three 2D section images followed by quantification of the synthetic 3D image..

Finally, those obtained microstructural features were input into XGBoost or neural network as descriptors to be correlated with extra-ordinally high hardness of the AM 316L steel. In addition, importance of those descriptors were evaluated by SHapley Additive exPlanation (shap) with XGBoost and sensitive analysis with neural network. This importance analysis was performed because of explainable AI.

*Keywords: HAADF-STEM, scale-bridging analysis, SliceGAN, generative adversarial network, additive manufacturing*

# Melt pool flow induced uniform dispersion of reinforcing particles in additively manufactured metallic composites

**Zan Li**[1], Y. Morris Wang[2]

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## Abstract

Additive manufacturing has gained increasing interest to fabricate metal matrix composites. Particle agglomeration remains a critical challenge and can severely compromise the mechanical properties, in particular tensile ductility. In this talk, we show that laser powder-bed-fusion (L-PBF) is able to uniformly disperse particles in metal matrices, taking advantages of particle flow dynamics during melting and remelting. We demonstrate our approach in a $TiB_2$ reinforced aluminum system and produce a high dispersion of fine $TiB_2$ particles (with sizes down to tens of nanometers) in a single print. Both micron- (1-5 μm) and nano-sized (40 nm) $TiB_2$ particles are found to be uniformly dispersed in composites, with a volume fraction of up to 25%. High-fidelity computer modeling indicates that although particles flow with Marangoni vortexes, the melt pool overlapping and subsequent re-melting/re-solidification play an important role for the successful dispersion. The propelling effect of vapor depression and particle filling via the Marangoni vortex flow are the two main mechanisms that lead to the uniform dispersion. We show that compared to composites with nonuniform particle dispersion, L-PBF aluminum 2024 composites have ~30% higher tensile strength and ~16% higher Young's modulus, together with a marked improvement of tensile ductility (up to three times higher).

*Keywords: Metal matrix composites; Dispersion; Laser powder-bed-fusion; Particle dynamics; Ductility*

# Effects of Laser Powder Bed Fusion (LPBF) process parameters on Ti6246 microstructure and mechanical properties

**Prince Valentine Cobbinah[1],** Sae Matsunaga[1], Yoshiaki Toda[2], Ryosuke Ozasa[3], Takuya Ishimoto[3,4,5], Masayuki Okugawa[3], Yuichiro Koizumi[3], Takayoshi Nakano[3,4], Yoko Yamabe-Mitarai[1]

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## Abstract

Microstructure development during the Laser Powder Bed Fusion (LPBF) process strongly depends on solidification parameters such as thermal gradient, undercooling, and solidification rate. The nature and degree of these solidification parameters hinge on the synergistic effects of the LPBF process parameters and the processed alloy's characteristics. However, the solid-state phase transformation ($\beta \rightarrow \alpha/\alpha'$) in titanium alloys such as Ti-6Al-2Sn-4Zr-6Mo wt.% (Ti6246) presents a challenge when processed by LPBF. Therefore, this study thoroughly investigates the influence of LPBF process parameters on phase and microstructure evolution and the attendant mechanical performance. Foremost, the laser power input and scan speed were optimized from 180 - 360 W and 600 - 1400 mm.s$^{-1}$, respectively, to build cylindrical samples. Two scan strategies were used: the bi-directional scanning in the X-axis without rotations in layers and the unidirectional scanning with 67° rotation in layers. Additionally, single-track simulation studies based on selected conditions were performed to determine the melting mode, melt pool shapes, and solidification parameters. The formed microstructures were observed in the plane normal to the scanning and transverse directions using the scanning electron microscope (SEM). Our results establish a relationship between the LPBF process parameters, the formed phase and microstructure, and the mechanical properties of Ti6246. In all, this study provides a rare insight into the LPBF processability of a $\beta$-stabilized $\alpha$+$\beta$ Ti alloy and is relevant for prospective structural applications.

*Keywords: LPBF, Ti6246, titanium, martensitic, acicular*

# Technical **Oral Session _ Session 10**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 10-2 (E10-2)** **09:00 - 10:15, Nov. 23**

**Chair :** Takuya ISHIMOTO (University of Toyama) 303A, 3F

09:00-09:15 **O-E0169** **Layered light-metals materials produced by a double spray forming machine**
Dmitri LOUZGUINE (Tohoku University, Japan)

09:15-09:30 **O-E0254** **Design strategy for eliminating cracking and improving mechanical properties of Al-Mg-Si alloys fabricated by laser melting deposition**
Wenzhe Li (Beijing Institute of Technology, China)

09:30-09:45 **O-E0465** **Mesoscopic chemical heterogeneities in laser powder bed fused CoCrMo and Ni mixed powders and their effect on the mechanical properties**
Siyuan Wei (Agency for Science, Technology and Research, Singapore)

09:45-10:00 **O-E0566** **Evaluation of physical properties of food ink for 3D food printers and three-dimensional noodle food modelling**
Fujiwara Koki (Yamagata University, Japan)

10:00-10:15 **O-E0816** **Post-processing technology of DLP-based additive manufacturing for 3D transparent yttria construction**
Sinuo Zhang (Korea Institute of Materials Science, Korea)

# Layered light-metals materials produced by a double spray forming machine

**Dmitri V. Louzguine**[1,2]

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## Abstract

A new additive manufacturing method of production of bulk/macroscopic double-layer metallic materials by using a unique Double Spray Forming machine in situ under a protective high-purity argon atmosphere will be presented. This method allows direct layer by layer deposition of metallic materials with good interlayer adhesion without formation of internal oxides [1]. The double-layered materials: Al / Mg, Al alloy / Mg alloy and Al alloy / Zr-based glassy (amorphous) alloy were produced. The resulting materials consist of a combination of a relatively hard layer 1 and a relatively soft layer 2, thus making in-situ layered composites. The obtained structures were examined by X-ray diffractometry and scanning electron microscopy. The proposed method can be applied for production of other double layer metallic materials including crystal/glassy ones and can be used by the scientists and engineers working in various research fields.

[1]. D. V. Louzguine-Luzgin, A. Watanabe, V. O. Semin, Double spray forming machine and its applications to layered light-metals materials production, Journal of Manufacturing Processes, 84 (2022) 727–733.

*Keywords: double spray forming; layered composite; X-ray diffractometry; scanning electron microscopy.*

# Design strategy for eliminating cracking and improving mechanical properties of Al-Mg-Si alloys fabricated by laser melting deposition

**Wenzhe Li**[1], Feng Qian[1, 2], Jinyue Li[1], Yichao Zhu[1], Yaojian Liang[1, 2], Shun Xu[1, 2], Yanjun Li[3], Xingwang Cheng[1, 2, 4]

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## Abstract

Laser-based additively manufactured Al-Mg-Si (6xxx) aluminum alloys have long suffered from coarse columnar grains and continuous hot cracks, which greatly limit their application. In this work, a novel and easy solution of adopting interlayer pause (IP) strategy is demonstrated to eliminate hot cracks and thus improve mechanical properties of the Al-Mg-Si alloys fabricated by laser melting deposition (LMD). It is found that increasing IP time not only facilitates the refinement of coarse columnar grains, but also inhibits the favoured grain growth tendency along building direction and induces the columnar to equiaxed transition. Additionally, an appropriate IP time is demonstrated to eliminate hot cracks along the columnar grain boundaries and reduce the number density of porosities; but further prolonging IP time results in the formation of a large number of long horizontal lath-like cracks. On the other hand, the extremely-rapid solidification during LMD inhibits the formation of primary intermetallic particles and further facilitates the precipitation of age hardening precipitates. With the optimal IP strategy of 8 s per layer, the LMDed AA6061 alloy exhibits a yield strength (YS) of 281 ± 1 MPa and an elongation of 18% after T6 heat treatment, showing even better mechanical properties than their cast and wrought counterparts. This IP strategy provides a guideline for future LMD manufacturing of high-strength wrought Al alloys (such as 2xxx and 7xxx alloys).

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: Additive manufacturing, Laser melting deposition, Interlayer pause, Aluminum alloys, Hot cracking*

# Mesoscopic chemical heterogeneities in laser powder bed fused CoCrMo and Ni mixed powders and their effect on the mechanical properties

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## Abstract

The conflict between the rapidly growing demand from the additive manufacturing industry and the currently limited materials library calls for high-throughput alloy screening method and design principles that makes full use of intrinsic features of the fabrication process. For the former, combination of in situ alloying and building compositionally graded alloy allows for rapid exploration of the compositions that has not been hitherto examined. For the latter, the inevitable formation of chemical heterogeneity during in situ alloying can be taken as a strengthening mechanism, instead of 'undesirable' defects. Despite the recent findings of heterogeneity induced strengthening in the additively manufactured metallic parts, how to turn the serendipity into reliable design principle is in urgent need of understanding, especially for single phase alloys. Here, CoCrMo alloy and Ni, which form stable face centered cubic structure and have similar melting point and disparate stacking fault energy, are chosen as an example system. Banded grain morphology and chemical segregation are created, and effect of micro-segregation on the mechanical properties is further studied. It is revealed that microscale chemical segregation can strengthen the matrix and improve the work hardening ability of the bulk material. These findings shed light on advancing the design principle in a broad class of additively manufactured alloys.

*Keywords: CoCrMo alloy; laser powder bed fusion; strengthening mechanism; heterogeneity; nanoindentation.*

# Evaluation of physical properties of food ink for 3D food printers and three-dimensional noodle food modelling

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## Abstract

Today, individual food preferences are becoming stronger in response to the diversification of food, and in the case of ramen restaurants, automated food delivery technology that can respond to individual orders for noodle consistency, such as firm, normal, or soft, has not yet been established. Therefore, we focused on food modelling using a food 3D printer, which is expected to make it easier to create food products according to individual tastes during the digitalization of food. We show a method for easily adjusting the texture of food products by using two different types of 3D food printers, a screw type, and a laser type, to create food products with different textures to suit individual needs. Ingredient ink is made from powder, water, and thickener, and after forming, it is heated by steaming or boiling. The following table shows the range of viscosity and hardness before and after modelling that can be modelled by each 3D printer. To change the texture of the modelled object, the infill of the modelling parameters, the shape of the modelled object, the laser irradiation time, etc. are changed and adjusted. In addition, by combining two types of 3D food printer models, the range of possible textures can be expanded.

*Keywords: 3D food printer, screw type, laser type, texture*

# Post-processing technology of DLP-based additive manufacturing for 3D transparent yttria construction

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## Abstract

Yttria ($Y_2O_3$) is a promising transparent ceramic with exceptional transparency, mechanical, and chemical properties, as well as high fracture toughness, hardness, and a high dielectric property making it suitable for various applications such as missile domes, scintillators, and optoelectronic devices in harsh environments. High-quality transparent Yttria ($Y_2O_3$) can be produced using various shaping techniques, including dry pressing, gel casting, and slip casting. However, the geometric control limits of shaping processes would hinder the utilization and application of transparent $Y_2O_3$. We herein propose digital light processing (DLP)-based additive manufacturing (AM) as one of the best solutions to this structural drawback. Transparent ceramics AM has lately gained popularity, however, it confronts issues due to limited transparency and printing resolution. In this study, 3D-structured transparent $Y_2O_3$ ceramic was achieved via DLP-based AM technology assisted by vacuum sintering, and the critical factors governing the transparency were revealed. As sintering additives, zirconia and lanthana were utilized to regulate grain growth. Printing parameters including layer thickness and UV light intensity were optimized to control printing accuracy. Following pre-sintering in air and vacuum sintering treatments, the transparent $Y_2O_3$ ceramics attained a high transmittance reaching 98.7% of the theoretical limit by achieving a fine-grained dense microstructure. Polished with newly developed 3D polishing technology, the 3D $Y_2O_3$ lens exhibits superior optical imaging capability. This study demonstrates that overcoming the geometric control limitation of $Y_2O_3$ by ceramic AM offers excellent promise for expanding the utilization of $Y_2O_3$ in various applications.

*Keywords: Additive manufacturing, Digital light processing, Transparent ceramics, Yttria*

# Technical **Oral Session _ Session 10**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 10 (K10)** **09:00 - 10:15, Nov. 23**

**Chair :** Masato Ohnuma (Hokkaido University) Samda Hall B, 3F

09:00-09:15 **O-K0977** **High-entropy alloy catalysts with hierarchical porous structures for efficient water electrolysis**
Xiong Jun Liu (University of Science And Technology Beijing, China)

09:15-09:30 **O-K0108** **Shape memory behavior of high-temperature high entropy shape memory alloys (HT-HESMAs) designed by DFT**
Yu Nien Shen (The University of Tokyo, Japan)

09:30-09:45 **O-K0127** **Elemental segregation and magnetic properties of the equimolar GdTbDyHoEr rare earth high entropy alloy**
Binbin Liu (University of Science and Technology Beijing, China)

09:45-10:00 **O-K0153** **Influence of Supporting Electrolyte LiClO4 on Synthesis of Film Containing CrMnFeCoNi by Electroplating in Organic Solvent**
Tian Xiao (Hiroshima Institute of Technology, Japan)

10:00-10:15 **O-K0892** **Fuzz evolution of Ti2ZrHfV0.5Mo0.2 refractory high entropy alloy under high-flux He ion irradiation**
Peng Zhang (Dalian University of Technology, China)

# High-entropy alloy catalysts with hierarchical porous structures for efficient water electrolysis

**Xiong-Jun Liu**[1], Zhibin Li[2], Zhao-Ping Lu[3]

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## Abstract

The development of renewable energy and the related conversion and storage technologies plays a crucial role in achieving the global goal of carbon neutrality. In particular, green hydrogen produced by water electrolysis with renewable electricity is regarded as one of the most promising pathways for solving the energy crisis and environmental issues in modern society. However, the sluggish kinetics of water-splitting reactions, namely, hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), remains a bottleneck to the water electrolysis technology. Although considerable 'fancy' electrocatalytic materials, such as nanoparticles, nanowires and nanosheets, have been developed in the lab, unfortunately, few of them can be readily utilized under industrial conditions. The main reason is that industrial sectors need catalysts to simultaneously meet the requirements of low cost, high activity, long-term durability and easy mass production. Recently, high entropy-alloys (HEAs) have been found to be of great potential as efficient catalytic materials for water electrolysis due to their compositional flexibility, structural stability, and strong alloying effects. In this talk, we will report our recent progresses in the development of HEA water-splitting catalysts based on physical metallurgy principles. Specifically, self-supported non-precious-metal-based HEA catalysts with hierarchical porous structures were mass-produced by modulating phase separation, spinodal decomposition or eutectic reaction. These HEA electrodes simultaneously exhibited superior activity and outstanding long-term durability towards alkaline HER and OER. The underlying mechanism responsible for the enhanced catalytic performance will be also discussed.

*Keywords: High entropy-alloys, Hierarchical porous structures, Water electrolysis, Green hydrogen*

# Shape memory behavior of high-temperature high entropy shape memory alloys (HT-HESMAs) designed by DFT

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## Abstract

Shape memory alloys (SMAs) such as TiNi have been attractive in a variety of fields due to their superior shape memory effect and super-elasticity. However, the current application of TiNi is limited to temperatures below 100 °C because of the low martensitic transformation temperature (MTT). Recently, we were able to increase the MTT by adding a variety of alloying elements to TiNi system. Furthermore, we have suggested and investigated new types of shape memory alloys such as TiPd and TiPt as the potential candidates for high-temperature SMAs which MTTs are in the range of 500 to 1000 ºC. However, these alloys showed small transformation strain, and exhibited unrecovered plastic deformation that leads to imperfect shape recovery. Therefore, improving of the high temperature strength of TiPd and TiPt is needed. Our past studies indicated that partially substituting Pd and Pt with different elements could improve the high temperature strength, its composition dependence is still not clear due to the lack of atomic-scale understanding. To deepen the understanding of the atomic scale, the martensite transformation with DFT-based first-principles calculations has been investigated. We selected seven alloys, $Ti_{43.5}Zr_{6.5}Pt_{30}Pd_{15}Co_5$, $Ti_{43.5}Zr_{6.5}Pt_{36}Pd_8Co_6$, $Ti_{45}Zr_5Pt_{19}Pd_{25}Co_6$, $Ti_{25}Zr_{25}Pd_{42.5}Co_{7.5}$, $Ti_{25}Zr_{25}Pd_{41}Co_9$, $Ti_{35}Zr_{15}Pd_{39}Co_{11}$, and $Ti_{27}Zr_{23}Pd_{40.5}Co_{9.5}$ as the candidates of the high temperature SMAs with good high temperature mechanical properties by utilizing the results of density functional theory (DFT) based first-principles calculations in which virtual crystal approximation (VCA) approach was employed to systematically track small composition variations. The experimental verification of the mechanical properties will be reported.

*Keywords: Shape memory alloy, High entropy alloy, DFT, Shape memory effect, Super-elasticity.*

# Elemental segregation and magnetic properties of the equimolar GdTbDyHoEr rare earth high entropy alloy

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**Abstract**

The rare earth based high entropy alloys (RE-HEAs) have single hcp structure and good magnetocaloric effect, which show potential applications in magnetic refrigeration. Previous studies mainly focused on the structure and magnetocaloric properties such as the magnetic entropy change ($-\Delta S_M$) and refrigerant capacity (RC), but elemental segregation and magnetic domain structure are seldom studied.

In this study, the equimolar GdTbDyHoEr RE-HEA was chosen to study microstructure evolution and magnetic properties in both as-cast and annealed states. STEM-EDS (Energy dispersive spectroscopy), STEM-EELS (Electron energy loss spectroscopy) and APT (Atom probe tomography) are introduced to investigate elemental segregation, while VSM (Vibrating sample magnetometer) and STEM-DPC (Differential phase-contrast) are performed to study magnetocaloric effect and magnetic domain structure, respectively.

Although XRD indicated single hcp structure for as-cast alloy and annealed samples when the annealing temperature was below 600°C, obvious elemental segregation occurred in the matrix. STEM-EDS did not show apparent elemental difference between the new phase and the matrix, but high-energy STEM-EELS suggested that the new phase is rich in Tb but depleted in Er. STEM-NBDPs (nano beams diffraction patterns) implied the transition from hcp structure of the matrix to fcc structure of the new phase. APT results further indicated that such segregation could be attributed to oxygen. STEM-DPC results exhibited total reverse magnetic domain structure between the new phase and the matrix, whereas both $\Delta S_M$ and RC improved in the annealed sample when compared with the as-cast counterpart.

*Keywords: High entropy alloy; Segregation; magnetocaloric properties; magnetic domain, APT; STEM-DPC.*

# Fuzz evolution of $Ti_2ZrHfV_{0.5}Mo_{0.2}$ refractory high entropy alloy under high-flux He ion irradiation

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## Abstract

Refractory high entropy alloys (RHEAs) have gained increasing attention in future fusion devices due to their remarkable defect suppression capabilities. In controlled fusion reactors, plasma-facing materials have to suffer continuous high flux helium (He) ion irradiations. During high flux He irradiation, He can generate vacancy-interstitial pairs by trap mutation mechanism even without cascade collision. In this study, $Ti_2ZrHfV_{0.5}Mo_{0.2}$ RHEA was irradiated with 50 eV $He^+$ under 1200 K to various fluences of $5\times10^{24}$ - $1\times10^{26}$ ions/$m^2$. In the irradiated RHEA, the growth and degradation of fuzz were observed, and the elements showed a clear distribution: the fuzz were mainly composed of Zr, Hf elements, Ti showed depletion in the subsurface layer, while V, Mo showed enrichment in this layer. The enrichment of V was anomalous since the sputtering thresholds for He of V and Ti are similar ($E_{Ti}$ = 24 eV, $E_V$ = 29 eV). Moreover, unlike the W fuzz growth process, the adatoms used to form fuzz in $Ti_2ZrHfV_{0.5}Mo_{0.2}$ were derived from the Zr, Hf atoms diffusing through the vacancy-solute exchange mechanism, rather than from the atoms formed by the loop-punching mechanism. The anomalous enrichment of V atoms and the different fuzz growth mechanism were attributed to different migration rates of different elements in the alloy under vacancy diffusion mechanism and the formation of V, Mo enriched band blocking the continued formation of prismatic dislocation loops mainly composed of V and Mo.

*Keywords: refractory multi-principal element alloy; He ion irradiation; fuzz evolution; element distribution*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 11

November 23

10:50-12:30

# Technical **Oral Session _ Session 11**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 11-1 (A11-1)** **10:50 – 12:35, Nov. 23**

**Chair :** To be announced Halla Hall A, 3F

10:50-11:05 **O-A0046** **Tailoring austenite stability and mechanical behaviors via compositional core-shell structure in advanced high strength steels**
Shichun Liu (Tsinghua University, China)

11:05-11:20 **O-A0477** **The effect of pre-strains on the temperature and deformation-induced martensitic transformation in austenitic steels**
Lingyu Wang (Northeastern University, China)

11:20-11:35 **O-A0281** **Crystallographical characteristics of deformation-induced martensite transformation in ultrafine grained metastable austenitic steel**
Yuanhong LIU (Kyoto University, Japan)

11:35-11:50 **O-A0326** **Identification of Fatigue Properties and Deterioration Mechanism in the Repeated Earthquake and Fire Situation**
Jae-Yeon Han (Changwon National University, Korea)

11:50-12:05 **O-A0196** **Controlling of Crystallography and Incomplete Transformation Characteristics in A Low-Carbon Low-Alloy Steel**
Binbin Wu (Harbin Engineering University, China)

12:05-12:20 **O-A0332** **Investigation of Low-Cycle Fatigue Deformation Behavior Based on Dislocation in FeMnAlC Lightweight Steel for Low-Pressure Turbine Blade at RT/200 °C**
Si Yeon Kim (Changwon National University, Korea)

12:20-12:35 **O-A1135** **Unveiling the Mechanisms behind Texture Gradient Formation and its Impact on Torsional Performance of Steel Wires**
Chunni Jia (Chinese Academy of Science, China)

| O-A0046 |

# Tailoring austenite stability and mechanical behaviors via compositional core-shell structure in advanced high strength steels

**Shichun Liu[1],** Jun Chai[1], Xinhao Wan[1], Zhigang Yang[1], Chi Zhang[1], Hao Chen[1*]

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**Abstract**

Metastable retained austenite (RA) plays an important role in mechanical behaviour of advanced high strength steels (AHSS) via transformation induced plasticity (TRIP) effects. However, conventional AHSS typically have chemically homogeneous RA grains with nearly uniform mechanical stability, resulting in limited work hardening and Lüders band formation during deformation. In this contribution, a unique compositional core-shell structured RA, where Mn atoms are gradually distributed with a low Mn content in the core and a high Mn content in the shell, is designed in a medium Mn steel (MMS) steel by a so-called Flash-Austenite Reversion Treatment (Flash-ART). The core-shell design enhances the thermal stability of austenite, resulting in a significantly higher fraction of RA compared to conventional ART samples. Furthermore, both ex-situ EBSD measurements and molecular dynamics simulations indicate that the compositional core-shell RA could stepwisely transform into martensite and thus persistent TRIP effects upon deformation, which could effectively relieve the strength-ductility trade-off of MMS. The heterogeneous mechanical metastability could significantly enhance strain-hardening capability of AHSS, and provides an opportunity to improve mechanical performance.

*Keywords: Advanced high strength steels, Flash annealing; Retained austenite; Core-shell structure; Lüders band*

# The effect of pre-strains on the temperature and deformation-induced martensitic transformation in austenitic steels

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## Abstract

The transformation induced plasticity (TRIP) effect in metastable austenitic steels has attracted much attention in past decades as it provides significant strengthening contributions. While most researches focused on the continuous martensitic transformation during quenching and straining, there is an increasing interest in the austenite stability after pre-straining. It is particularly important for components that are firstly cold formed and then used in cryogenic and/or heavy-duty applications where extra thermal and deformation stimulations are present. In this contribution, we use a series of in-situ/quasi in-situ characterization techniques to probe the temperature and deformation-induced martensitic transformation in pre-strained austenitic steels. We reveal a common relationship between microstructural defects induced by the pre-strain and the growth restriction of martensite laths. Specifically, it is found that small pre-strains increase the defect densities and promote martensitic transformation whereas large pre-strains introduce much denser slip bands that hinder the growth of martensite. As a result, large pre-strains result in much lower martensite formation and enhanced variant selection. The same trend applies to both temperature and deformation-induced martensitic transformation. In addition, the effect of pre-strains on the subsequent transformation behaviour in both quasi-static and high-speed tensile tests are revealed and compared. A unified model describing both temperature and strain-induced martensitic transformation in pre-strained metastable austenite is presented.

*Keywords: Metastable austenite, Pre-strained austenite, Martensitic transformation, Thermal stability, Mechanical stability.*

# Crystallographical characteristics of deformation-induced martensite transformation in ultrafine grained metastable austenitic steel

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**Abstract**

An ultrafine grained Fe-24Ni-0.3C metastable austenitic steel fabricated by high-pressure torsion with subsequent annealing was subjected to uniaxial tension at room temperature to investigate the characteristics of deformation-induced martensitic transformation of the material. Microstructures of the specimen deformed to different tensile strains were observed by scanning electron microscope equipped with electron back-scattered diffraction (SEM-EBSD). It was confirmed that the volume fraction of deformation-induced martensite increased with increasing the tensile strain. During the tensile deformation, austenite exhibited a strong texture of <111>$_{fcc}$//tensile axis (TD) while the intensity of the <001>$_{fcc}$//TD component greatly decreased with the tensile strain, suggesting that the <001> oriented austenite grains had strong tendency to transform into martensite. Such crystallographical orientation dependence of the mechanical stability of austenite was interpreted by the Schmid factor of the shear system for martensitic transformation. Additionally, it was found that the number of martensite variants within each austenite grain was greatly limited in the ultrafine grained specimen, compared with that in the coarse-grained specimen. The effect of grain size on the deformation induced martensitic transformation will be discussed in detail in the presentation.

*Keywords: Deformation-induced martensite transformation, crystallography, ultrafine grain, metastable austenitic steel*

**Topic:** Symposium A - Advanced Steels and Properties

# Identification of Fatigue Properties and Deterioration Mechanism in the Repeated Earthquake and Fire Situation

**Jae-Yeon Han[1],** Cheol-Hyeok Yang[2], Joonoh moon[3], Chang-Hoon Lee[4], Jun-Ho Chung[5], Hyun-Uk Hong[6,*]

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## Abstract

As the frequency and damage of earthquakes in Korea are increasing and the dangerousness of post-earthquake fire (PEF) is emphasized, it is necessary to develop a high-performance H-beam with both earthquake/fire resistance characteristics. This study examined the correlation between microstructure and earthquake/fire resistance by adding alloy elements to two steel materials, A (0.31Mo-0.03Ti-0.021Nb) and B (0.2Mo-0.13Ti-0.001Nb). Steel A, with high Mo and Nb content, had a bainite structure, while steel B, with high Ti content, had a ferrite structure. In tensile results at room-temperature and 600℃ steel A satisfied both earthquake and refractory steel standards, while steel B did not meet the refractory steel standard due to a large decrease in yield strength at 600℃ compared to room temperature. Low-cycle fatigue results showed that steel A had superior fatigue characteristics compared to steel B, and TEM analysis revealed dislocation recovery and rearrangement, resulting in increased fatigue life. For bainite steel with seismic/fire resistance, a combination of room-temperature low-cycle fatigue test and heat exposure was used to evaluate the soundness of H-beams in terms of reuse and maintenance. After the heat exposure, additional MX precipitates were formed, and a cyclic softening due to the dislocation annihilation was identified as the fatigue cycles progressed. And despite the repeated deterioration process, a fatigue life similar to that of a simple low-cycle fatigue test was confirmed. These results confirm that the bainite steel formed by adding Mo and Nb satisfies both seismic/fire resistance properties and is effective in terms of reuse and maintenance.

*Keywords: Seismic property, Fire property, Bainite, MX precipitates, Low Cycle Fatigue*

# Controlling of Crystallography and Incomplete Transformation Characteristics in A Low-Carbon Low-Alloy Steel

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Intermediate temperature transformation products, including bainite ferrite (BF), acicular ferrite (AF) and martensite-austenite (M-A) islands, are very common in the field of welding. The toughness of welding seam and heat-affected zone (HAZ) is closely related to the crystallography characteristics of matrix and M-A islands. In this study, we found that the crystallography characteristics of matrix and M-A islands can be regulated through nucleation intervention. The introduction of intermediate annealing treatment (IAT) after austenitizing treatment can promote the segregation of more boron (B) and molybdenum (Mo) elements at prior austenite grain boundaries (PAGBs) and the formation of film-like allotriomorphic ferrite, thereby impeding the nucleation at PAGBs. At the same time, the intragranular ferrite embryos formed in the IAT grow rapidly in the subsequent transformation to form acicular ferrite. Acicular ferrite can be formed under the condition of ultra-fast cooling rate, which can significantly improve the low-temperature impact toughness. In addition, the kinetics of isothermal transformation is accelerated by the introduce of acicular ferrite, thereby increasing the density of the packet boundaries and optimizing the structure of martensite-austenite (M-A) islands.

# Investigation of Low-Cycle Fatigue Deformation Behavior Based on Dislocation in FeMnAlC Lightweight Steel for Low-Pressure Turbine Blade at RT/200 °C

**Si-Yeon Kim[1],** Ui-Seok Ko[2], Chi-Won Kim[3], Seong-Jun Park[4] and Hyun-Uk Hong[5]

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## Abstract

In response to social and economic demands for improved efficiency and reduced carbon emissions in the power generation industry, research efforts are focusing on high-specific strength materials, with FeMnAlC alloy-based lightweight steel. Fatigue properties are critical when considering the application environment of low-pressure turbine blades for power generation. Consequently, this study aims to analyze the low-cycle fatigue behavior of FeMnAlC lightweight steel materials for low-pressure turbine blade applications. The alloy examined in this study is an austenitic lightweight steel, Fe-22Mn-8Al-0.9C. Following solution heat treatment, the material was aged at 550°C for 6 hours to induce the precipitation of κ-carbide, a key reinforcement factor for lightweight steel. The resulting microstructure featured approximately 10 nm finely precipitated κ-carbide within the austenite matrix. Low-cycle fatigue tests revealed cyclic softening at room temperature and cyclic hardening at 200°C under all conditions within a strain range ($\Delta\varepsilon t$) of 0.6 to 2.0%. Additionally, unlike at room temperature, the serrated flows were observed in the hysteresis loop at 200°C. Due to these results, the reason for cyclic hardening is thought to be DSA. To identify cyclic hardening due to DSA, further low-cycle fatigue tests were conducted at various temperatures (from room temperature to 400°C). To discern cyclic softening, dislocation behavior by cycle was observed under a total strain range ($\Delta\varepsilon t$) of 1.4%, with a low-cycle fatigue life of 5,000 cycles at room temperature. This analysis considered the dislocation evolution during low-cycle fatigue deformation of the alloy and the correlation between cyclic softening and cyclic hardening.

*Keywords: Lightweight steel, Low-cycle fatigue, DSA, Glide plane softening*

# Unveiling the Mechanisms behind Texture Gradient Formation and its Impact on Torsional Performance of Steel Wires

**Jia Chunni**[1], Wang Pei[1], Li Dianzhong[1]

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## Abstract

Cold-drawn pearlitic steel wire possesses extremely high strength, making it the strongest steel product currently available. Due to its excellent mechanical properties, cold-drawn steel wire is widely used in industrial production. However, due to the nature of the drawing process itself, the deformation along the cross section of the steel wire is highly non-uniform. This work aims to reveal the macroscopic texture gradient formation mechanism along the cross section. A finite element model based on macroscale was established to simulate the deformation behaviour of pearlite wires during cold drawing, with the purpose of making a thorough inquiry of inhomogeneous elastic-plastic deformation behaviour. The macro mechanical responses are incorporated into the meso scale representative volume element (RVE) model as boundary conditions, with the aim of conducting a comprehensive investigation on the effect of inhomogeneous deformation characteristics on the texture formation. The influence of non-uniform texture distribution on the subsequent torsional behaviour of steel wire was further investigated and discussed. The results indicate that the non-uniform texture distribution of the steel wire should be attributed to multiaxial stress state across the cross-section. At the center of steel wire, the maximum principal stress aligns with the drawing axis, with a dominant <110> fiber texture. Conversely, in proximity to the surface, the maximum principal stress orientation progressively shifts towards the circumferential direction, accompanied by an evolving texture characterized by {110}<110> radial orientation. The {110}<110> circular texture weakened the torsion ability of the wires given that the limited slip systems are activated.

*Keywords: Steel wire drawing; Texture; Torsion; Pearlite steel; Crystal plasticity.*

# Technical **Oral Session _ Session 11**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 11-2 (A11-2)** **10:50 – 12:35, Nov. 23**

**Chair :** Jae Sang Lee (Pohang University of Science and Technology) 303B, 3F

10:50-11:05 **O-A0194** **Investigation of tensile and fatigue properties of 316L stainless steel at 20K**
Chetan Singh (Chungnam National University, Korea)

11:05-11:20 **O-A0009** **Development of hot dip galvanized TBF steel with a tensile strength of 980MPa**
Yinghua Jiang (Research Institute of Technology, Shougang Group Co., Ltd, Korea)

11:20-11:35 **O-A0764** **Cyclic deformation behavior of high manganese steels at ultra-low temperature**
SUJITH S V (Chungnam National University, Korea)

11:35-11:50 **O-A0077** **Effect of Tempering Temperature on Microstructure and Mechanical and Magnetic Properties of Ultra-High Strength Rim Sheet Steel**
Chang Song (Baosteel Central Research Institute, Wuhan Iron & Steel Co., Ltd., China)

11:50-12:05 **O-A0079** **Influence of Cooling Parameters on Precipitation of Grain Boundary Cementite of 0.92%C Steel Wire Rods**
Hang Gao (Ansteel Group, China)

12:05-12:20 **O-A0088** **Effect of Different Heat Treatment Temperatures on Microstructure and Precipitated Phase in Advanced High Strength Steel**
Wang Bo (Hebei University of Science and Technology, China)

12:20-12:35 **O-A0117** **A Comprehensive Study of HER in Complex Phase and Martensitic Steels: Understanding the Role of Punching Damage**
Cho Woojin (Seoul National University, Korea)

# Investigation of tensile and fatigue properties of 316L stainless steel at 20K

**Chetan Singh**, You Sub Kim, Soo Yeol Lee

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**Abstract**

Stainless steel 316L (SS316L) is widely used in cryogenic applications due to its excellent mechanical properties and corrosion resistance. However, the mechanical behavior of this material at cryogenic temperatures is not well understood, especially at temperatures below 77 K. In this study, we investigated the tensile and fatigue behavior of hot-rolled SS316L stainless steel at room temperature and 20K. The tensile test conducted provided insights into the effect of temperature on the mechanical properties of SS316L under quasi-static loading conditions. The findings demonstrated that lowering temperature increased yield strength and tensile strength and decreased uniform elongation. Moreover, unusual deformation, which is a serration phenomenon, was observed. On the other hand, fatigue tests performed using constant amplitude loading and variable loading conditions provided valuable insights into the effect of temperature on the mechanical properties under dynamic loading conditions. Fractographic analysis conducted on the samples tested provided a crucial understanding of the failure mechanisms. The current work will provide important implications for the design and operation of cryogenic equipment under static and dynamic loading conditions.

*Keywords: SS316L, fatigue behavior, ultra-cryogenic temperature*

# Development of hot dip galvanized TBF steel with a tensile strength of 980MPa

**Yinghua Jiang[1, 2],** Feng Yang[1,2], Huasai Liu[1,2], Yun Han[1,2]

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## Abstract

In the present work industrial trials for TBF steel with a minimum tensile strength of 980MPa produced via a continuous hot-dip coating of AHSS are discussed in detail. Dilatometry was employed to investigate the phase transformation characteristics of the cold rolled materials by isothermal transformation and continuous cooling experiments. In addition annealing simulations were carried out to investigate the microstructure and mechanical properties as a function of quenching temperature.The successfully produced industrial coils with the microstructure consisting predominantly of the lath-shaped bainitic/tempered martensite matrix and inclusions of lamellar retained austenite exhibit excellent mechanical properties.

*Keywords: Quenching temperature; Bainite; Mechanical properties; Retained austenite*

# Cyclic deformation behavior of high manganese steels at ultra-low temperature

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## Abstract

The storage and transportation of liquefied natural gas (LNG) is increasingly important, but technologically challenging. With appropriate strengthening mechanisms, high manganese austenitic steel offers a promising combination of mechanical properties and cost comprising excellent toughness at cryogenic temperature. In the present investigation, high manganese steel consisting of ~26Mn, in which the ε-martensite transformation was almost suppressed, were used. For the critical industrial applications of high manganese steels, the ultra-low temperature (~ 20K) mechanical response was not examined on these steels till date. The most relevant studies including tensile properties, crack tip opening displacement (CTOD) and fatigue response under different loading conditions were examined. More specifically, the effects of stress amplitude and frequency on the fatigue life of high manganese steel were examined at room temperature and ultra-low temperature of 20K. For fatigue response, results were elaborated by a stress life method under fluctuating stress. The S–N fatigue and the fatigue crack propagation behaviours of high manganese austenitic steels were discussed based on the microscopic crack propagations and their mutual interactions. Further, the elastoplastic fracture toughness, micro mechanisms and microstructural features with J-R curves were obtained by using compact-tension (CT) specimens. The unloading compliance method was applied to measure crack extension. In addition to the above, the microstructural analysis of the stable crack growth zones in the fractured CT specimens allowed the fundamental identification of various crack propagations which is important in deciding the load carrying capacity of the above steels.

*Keywords: High cycle fatigue, Mechanical properties, Fracture, Fatigue strength.*

# Effect of Tempering Temperature on Microstructure and Mechanical and Magnetic Properties of Ultra-High Strength Rim Sheet Steel

**Song Chang**[1], He Ya-Yuan[2], Du Ming[3], Liu Zhiyong[4]

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## Abstract

In order to develop the ultra-high strength rim sheet steel, the effect of tempering temperature on the microstructure and properties of experimental steel was investigated . The results show that with the increase of tempering temperature, the yield strength gradually increases first and then decreases. At tempering temperature 400 ℃, the experimental steel shows the best properties with yield strength of 1150 MPa, elongation of 16%, Charpy impact energy at -40℃ of 77 J. The magnetic induction reaches the lowest value as quenched and then increases with the of tempering temperature, which tends to be stable after being tempered at 400~450℃.

*Keywords: Provide a maximum of 5 keywords which appropriately represent the contents of the presentation.*

# Influence of Cooling Parameters on Precipitation of Grain Boundary Cementite of 0.92%C Steel Wire Rods

**Hang Gao**[1,2], Dayong Guo[1,2], Yang Pan[1,2], Bo Zhang[1,2], Liguo Ma[1,2], BingXi Wang[1,2]

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## Abstract

Drawability is an important property of cord steel wire rods to ensure the productivity of steel wire. The grain boundary cementite(GBC) has harmful influence on the drawability of steel, which is normally strongly related to carbon content, center segregation and cooling rate after laying. Because of the high carbon content and existence of severe center segregation, the control of GBC of 0.92%C steel wire rods usually requires a high cooling rate, which leads to high strength and low drawability. Thus a new method is needed to prevent the precipitation of GBC. In this paper, the influence of deforming and cooling parameters on precipitation of GBC of 1.15%C steel was studied. The carbon content corresponds to 0.92%C wire rods with a center segregation index 1.25. The results show that the cementite precipitation temperature range of specimens without deformation decreases from above 950℃ to 900℃-950℃ compared to specimens with compression of 30%. The reason is that the specimens without deformation has lower energy inside the austenite due to bigger grain size and less crystal defects like dislocations etc., the cementite precipitation temperature is delayed to a lower range which decreases the growing rate and amount of GBC. Therefore, a higher laying head temperature and longer holding time in high temperature range was applied to the industrial experiment of 0.92%C wire rods to fully release the deformation energy accumulated in the rolling to prevent the precipitation of GBC. The penalty point of GBC decreased dramatically from 42 to 22.

*Keywords: high-carbon steel wire rods, segregation, GBC, precipitation temperature*

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# Effect of Different Heat Treatment Temperatures on Microstructure and Precipitated Phase in Advanced High Strength Steel

**Di Zhang[1],** Yinzhao Liu[2], Huilan Sun[3], Bo Wang[4], Cheng Ma[5]

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**Abstract:**

The effects of different homogenization temperatures on the microstructure and precipitates of medium manganese steel billet in Fe-0.2C-12Mn-3Al-3Ni-2Cu system were studied by means of optical microscope, electron scanning microscope and Vickers hardness. The results show that the contents of austenite and martensite with island distribution increase after different heat treatment temperatures, among which the microstructure at 1200 ℃ is the most uniform and the influence on grain coarsening is low. In addition, this condition can not only retain the dispersed spherical precipitates in the original sample, but also obtain more uniform hardness, which is conducive to the subsequent hot rolling process.

*Keywords:* different homogenization temperatures; medium manganese steel billet; microstructure; spherical precipitates; hot rolling

# A Comprehensive Study of HER in Complex Phase and Martensitic Steels: Understanding the Role of Punching Damage

**Woojin Cho**[1], Byeong-Seok Jeong[2], Seung-Ho Lee[3], Minwoo Park[4]
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## Abstract

This study suggests a new concept for understanding the hole expansion ratio (HER) of complex phase (CP) and martensitic (MT) steels before and after heat treatment at 400°C for 20 minutes. Prior to conducting the hole expansion test, holes were fabricated using two methods: electrical discharge machining (EDM) and punching. EDM was used as it results in minimal damage at the hole vicinity. The HER obtained from the EDMed-hole was referred to as $HER_0$ and showed a strong correlation with uniaxial tensile properties. The HER obtained from the punched-hole was referred to as $HER_p$ and was lower than $HER_0$ due to significant damage accumulated during the punching process. The changes in $HER_0$ and $HER_p$ after heat treatment showed different trends for CP and MT steels. After heat treatment, the CP steel exhibited an increase in both $HER_0$ and $HER_p$, while the MT steel showed a decrease in $HER_0$ but an increase in $HER_p$. We propose that $HER_p$ is determined by $HER_0$ and punching damage. In CP steel, there was little difference in punching damage before and after heat treatment, resulting in a consistent increasing trend in $HER_0$ and $HER_p$ after heat treatment. On the other hand, in MT steel, tempering embrittlement caused by heat treatment decreased $HER_0$, but it also significantly reduced the punching damage. This explains the increase in $HER_p$ after heat treatment. These results demonstrate the validity of the approach to understanding $HER_p$ through $HER_0$ and punching damage. (240 words)

*Keywords: Hole expansion ratio; Complex Phase steel; Martensitic steel; Tempering embrittlement;*

# Technical **Oral Session _ Session 11**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 11-1 (D11-1)** **10:50 -12:25, Nov. 23**

Chair : Yoshihito Kawamura (Kumamoto University)
Yan Yang (Chongqing University)

Samda Hall A, 3F

10:50-11:10 **I-D0677** **[Invited] TD-split Texture Evolution during Thermo-Mechanical Treatment in Mg Alloy Sheets**
Byeong-Chan Suh (Korea Institute of Materials Science, Korea)

11:10-11:25 **O-D0024** **Towards the development of room temperature formable magnesium alloy sheets**
Mingzhe Bian (National Institute Of Advanced Industrial Science And Technology (AIST), Japan)

11:25-11:40 **O-D0610** **Twinning and detwinning in AZ31 alloy at 20K studied by in-situ neutron diffraction**
Wu Gong (Japan Atomic Energy Agency, Japan)

11:40-11:55 **O-D0125** **Orientation dependence of active non-basal slips in pure magnesium single crystals**
Shinji Ando (Kumamoto University, Japan)

11:55-12:10 **O-D0708** **Three-dimensional Shape and Stress Field of a Deformation Twin in Magnesium**
Hong Liu (Shanghai Jiao Tong University, China)

12:10-12:25 **O-D0802** **Multi-Step processing approach to tailor texture for achieving ultrahigh strength and ductility in 2Al-1Zn-1Ca Magnesium Alloy**
HAFIZ MUHAMMAD REHAN TARIQ (Incheon National University, Korea)

# TD-split Texture Evolution during Thermo-Mechanical Treatment in Mg Alloy Sheets

Ying Ma[1], Seoung-Yoon Yu[2], Jae H. Kim[3],
Young Min Kim[4], Nack J. Kim[5], **Byeong-Chan Suh[6]**

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## Abstract

A lot of effort has been made to broaden the applications of Mg alloy sheets in industries. In particular, a lot of research has been conducted to improve formability, which is one of the critical issues in Mg alloy sheets. As a result, some Mg alloy sheets containing Ca/RE elements with Zn element show comparable stretch formability to that of Al alloys. Their excellent formability is mainly due to a formation of weak TD-split texture during thermo-mechanical treatment. However, the detailed mechanisms responsible for such texture evolution are not clearly understood, yet. This presentation covers the recent researches on the development of Mg alloy sheets having high formability and the evolution mechanism of such a TD-split texture in those alloys. Especially, the microstructural and texture evolution during annealing in Mg alloy sheets showing TD-split texture has been analysed by the direct observation of microstructure and simulation by strain-induced boundary migration (SIBM) modelling. It clearly demonstrates that the TD-split texture is mainly due to a formation of TD-broad texture during rolling and consequent recrystallization by SIBM.

*Keywords: Mg alloy sheets, Texture, SIBM, Thermo-mechanical treatment*

| O-D0024 |

# Towards the development of room temperature formable magnesium alloy sheets

**Mingzhe Bian**[1], Xinsheng Huang[2], Yasumasa Chino[3]

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## Abstract

Magnesium (Mg) is the lightest structural metal; its density is about 1.74 g/cm$^3$, which is two-thirds that of aluminum and one-fourth that of steel. In addition, it has high thermal conductivity, high damping capacity, and good biocompatibility, which have attracted considerable interest over the past two decades for potential use in diverse applications. However, owing to the limited number of independent slip systems originating from their hexagonal close-packed crystal structure and the development of a strong basal texture during thermomechanical processing, Mg alloys usually exhibit poor formability at room temperature (RT). Development of new alloys and/or optimization of processing parameter have been shown to be effective ways to weaken the strong basal texture, and thus lead to a substantial improvement in the RT formability. In this talk, we will report the recent research progress in improving the RT formability of pure Mg by parts-per-million-level alloying and flame-retardant high-calcium-containing alloy by high temperature final rolling.

*Keywords: Magnesium alloys; rolling; formability; texture; enthalpies of mixing; grain boundary segregation.*

# Twinning and detwinning in AZ31 alloy at 20K studied by *in-situ* neutron diffraction

**Wu Gong[1],** Stefanus Harjo[1], Takuro Kawasaki[1], Kazuya Aizawa[1], Nobuhiro Tsuji[2]

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**Abstract**

Extension twinning and detwinning play crucial roles in deformation, particularly in cyclic loading deformation of magnesium (Mg) and its alloys. Due to the high potential for use in various applications, Mg products are inevitably subjected to cyclic loading and loading in various orientations at cryogenic temperatures in some cases. However, studies of deformation behavior in Mg alloys at such temperatures are limited, and the corresponding deformation mechanisms are far from fully understood. The present study investigated the cyclic loading-unloading behavior in a commercial AZ31 alloy (Mg-3wt.%Al-1wt.%Zn) at 20K and 298K using *in-situ* neutron diffraction. The volume fraction of twins and lattice stresses of twins and matrix during compression and unloading were quantitatively evaluated for revealing the temperature dependence of twinning and detwinning behavior in AZ31 alloy.

*In-situ* neutron diffraction experiments were conducted by a time-of-flight engineering neutron diffractometer "TAKUMI" at J-PARC. A commercial as-extruded AZ31 alloy (with 3 wt.% Al, 1 wt.% Zn and balance Mg) was used in the present study. Cylinder specimens with 8 mm in diameter and 16 mm in length were prepared with the loading direction aligned parallel to the extrusion direction. *In-situ* neutron diffraction experiments were conducted during cyclic compression and unloading at 21K and 298K. The strain was measured using an extensometer that spanned the irradiated region. Additionally, EBSD measurements were carried out to observe the microstructure changes of the specimens before and after deformation.

The yield stress and flow stress in the plastic regime up to 6% strain at 21K were slightly higher than those at 298K. However, the hysteresis loops (i.e., recovery strains) of the loading-unloading at 21K were significantly larger compared to those at 298K. The alternate increase and decrease in the integrated intensity of diffraction reflections confirmed the activity of twinning and detwinning corresponding to compressive deformation and unloading steps. During compression, twinning was more prevalent at 21K than that at 298K. A decrease in the volume fraction of twins and lattice stress relaxation were observed in each unloading step, which can be attributed to detwinning. The amount of detwinning and lattice stress relaxation were found to be higher at lower temperatures, which is considered to be the origin of the large recovery strain observed at 20K.

*Keywords: Magnesium; Neutron diffraction; Twinning; Detwinning; Cryogenic deformation.*

# Orientation dependence of active non-basal slips in pure magnesium single crystals

**Shinji Ando[1]**, Kento Mitani[2], Masato Sakai[3], Hiromoto Kitahara[4]

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## Abstract

According to von Mises, activation of non-basal slips is required in deformation of HCP crystals. To clarify active non-basal slip systems in magnesium, tensile tests of pure magnesium single crystals with various tensile axes parallel to basal plane were carried out at room temperature. In [11-20] tensile, {11-22}<11-23> second order pyramidal <c+a> slips (SPCS) occurred at yielding. {10-11}<11-23> first order pyramidal <c+a> slips (FPCS) also appeared at higher stress. When the tensile axes were tiled 20° and 25° from [10-10], singe crystals were deformed by SPCS as same as in [11-20] tensile. When the tensile axes were tiled 10° and 15° from [10-10], FPCS occurred at yielding and SPCS were slightly observed. When the tensile axes were tilted 6° from [10-10] and [10-10], single crystals brittlely fractured and no slip lines were observed. Critical resolved shear stress (CRSS) of SPCS gradually decreased with increasing tilt angle of tensile axis from [10-10]. In contrast, CRSS of FPCS increased with increasing the tilt angle and showed strong orientation dependence. In TEM observation, <a>, <c> and <c+a> dislocations were confirmed. <c+a> edge dislocations of SPCS were dissociated into <c> and <a> dislocations by thermal activation, then <c> dislocations parallel to the basal plane were formed. On the other hand, <c+a> screw dislocations could be dissociated by shear stress on prismatic plane. <c> dislocations non-parallel to the basal plane would be formed by the dissociation. Variation of active non-basal slips by the dissociation of <c+a> dislocations was discussed.

*Keywords: Pyramidal slip, Prismatic slip, CRSS, Slip lines, <c+a> dislocation*

# Three-dimensional Shape and Stress Field of a Deformation Twin in Magnesium

**H. Liu**[1], F. X. Lin[2], N. Moelans[3], L. M. Peng[1], J. F. Nie[4], I. J. Beyerlein[5,6]

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## Abstract

While the three-dimensional (3D) shape and stress field of a twin in hexagonal close-packed (HCP) metals have attracted considerable interest in recent years due to their substantial impact on internal stress and mechanical properties, a detailed understanding of their variation with twin size is still lacking. An analytical model that is not restricted by spatial scale is developed in this work by considering the effects of anisotropic boundary energy, elastic strain energy and plastic relaxation to predict the 3D shape with the minimum energy, and the stress field, of an isolated ellipsoidal twin of different sizes. The model is applied to Mg with a focus on the $\{10\bar{1}2\}$ twin type. The analytical results show that the nucleation of the nano-sized twin embryos is facilitated by the stress field near structural defects such as dislocations. During the expansion of this nano-sized twin embryo, the interplay between the elastic strain energy and interfacial energy changes the length of the twin along the twin shear (forward) direction from being shorter to longer than that along the lateral direction. In contrast to the current understandings, the maximum shear stress on the twin plane along the twin shear direction occurs at the lateral, rather than the forward, side of the twin. At the forward side, the maximum shear stress occurs at a distance ahead of the twin tip and this distance increases with increasing twin thickness.

*Keywords: Eshelby's theory, Nucleation, Morphology, Stress field, Plastic deformation*

# Multi-Step processing approach to tailor texture for achieving ultrahigh strength and ductility in 2Al-1Zn-1Ca Magnesium Alloy

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## Abstract

The performance of Mg alloys can be significantly enhanced by inducing {10-12} extension twinning. This strategy effectively modifies the crystallographic distribution along the <c-axis> in wrought Mg alloys, resulting in a notable decrease in plastic anisotropy [1]. Pre-twinning is a significant deformation mechanism that has the ability to activate ~86.3° lattice rotation and produce a new texture component that can entail synergetic improvements in strength and ductility [2, 3]. The objective of this work is to modify the texture of a 2Al-1Zn-1Ca magnesium alloy in order to attain ultrahigh strength and ductility. Accordingly, in this research, the microstructure and texture of the alloy were altered by combining cryogenic pre-stretching (5% at -170°C) followed by low-temperature annealing (170°C for 90 min) treatments. Hereafter, the processed sample will be called PSCA. After processing, microstructural and textural examination showed a twinned microstructure with a split basal texture. In comparison to the mechanical properties of as manufactured sample (Yield Strength (YS) – 170.5 MPa, Ultimate Tensile Strength (UTS) – 252 MPa, Elongation (EL) – 16.5%), PSCA sample had better mechanical characteristics, including ultra-high yield strength and increased strain to fracture (YS – 194 MPa, UTS – 267 MPa, EL – 21%). The weakening of the basal texture and the appearance of various twinning variants in individual grains leads to twin-twin interactions in PSCA sample, hence causing higher yield strength and excellent strain to failure. Another factor that took part in improving yield strength of PSCA sample is higher dislocation accumulations at grain boundaries that confirmed grain boundary (GB) strengthening effect [4].

*Keywords: Cryogenic Pre-straining, Annealing strengthening, Mg Alloy, Twin Variants, Texture*

# Technical **Oral Session _ Session 11**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 11-2 (D11-2)** **10:50 -12:25, Nov. 23**

**Chair :** Ma Qian (RMIT University), Seong-Woong Kim (Korea Atomic Energy Research Institute) **301, 3F**

10:50-11:20 **K-D0211** **[Keynote] Enhanced superplastic formability of a (α+β) Ti alloy with the metastable fine microstructure**
Hiroaki Matsumoto (Kagawa University, Japan)

11:20-11:50 **K-D0629** **[Keynote] Microstructural dependence of strength and toughness of a high-strength metastable beta titanium alloy**
Qiaoyan Sun (Xi'an Jiaotong University, China)

11:50-12:10 **I-D0255** **[Invited] Mechanical properties and twinning-induced plasticity of metastable β-type Ti alloys**
Ken Cho (Osaka University, Japan)

12:10-12:25 **O-D0511** **Microstructure evolution and strength-toughness of Ti2AlNb based alloy during across B2 forging**
Jianwei Xu (Northwestern Polytechnical University, China)

# Enhanced superplastic formability of a (α+β) Ti alloy with the metastable fine microstructure

**Hiroaki Matsumoto**[1]

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## Abstract

This work suggests the methodology for the enhancement of superplastic properties of a (α+β) Ti alloys (such as Ti-6Al-4V(Ti-64) and Ti-6Al-2Sn-4Zr-2Mo-Si (Ti-6242S) alloys) by means of the microstructural control of metastable microstructures such as a supersaturated fine-grained-α formation and an α′ martensite.

1) Ti alloys (Ti-64 and Ti-6242S) with an ultrafine-grained microstructure ($d_\alpha$=0.4 μm) consisting of a single supersaturated α phase exhibits low-temperature (below 700°C)–high-strain-rate ($10^{-2}$ $s^{-1}$) superplastic behavior. Herein, the β-phase precipitation, which is accelerated during the deformation, acts as an accommodation mechanism and contributes to the enhancement of superplasticity.

2) the Ti alloy having an α′ martensite microstructure exhibits a lower flow stress and a higher ductility in high temperature deformations (tested ranging from 700°C to 900°C) than those of the alloy with an equilibrium (α+β) microstructure. During deformation, the discontinuous dynamic recrystallization (DDRX) occurred from the α′ martensite acts as an additional accommodation mechanism, resulting in a higher ductility associated with the enhanced grain boundary sliding.

Quantitative analysis of deformation modes analyzed by internal variable theory indeed reveals that the fraction of grain boundary sliding activity is higher for the Ti alloys with metastable microstructures than that of the alloys with equilibrium (α+β) microstructures.

*Keywords: Titanium alloys, metastable microstructure, α′ martensite, supeplasticity, grain boundary sliding*

# Microstructural dependence of strength and toughness of a high-strength metastable beta titanium alloy

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## Abstract

Titanium alloys with high strength and toughness play an important role in reduction weight and increase reliability of machine parts in aeronautical industry. In present study two kind of microstructures, bimodal microstructure and lamellar structures were obtained by design heat treatment. The effect of aging temperature on the microstructures, strength and toughness is investigated in detail. The combination of strength and plasticity and toughness is discussed based on features of microstructures and the strengthening and toughening mechanism are discussed. The high strength is due to hinderance from alpha/beta phase against movement of dislocation and toughness in lamellar structure is attributed to low back stress in the tensile deformation. The results also exhibit that bimodal microstructural possesses good combination of strength and ductility and lamellar structure microstructure possesses excellent combination of strength and fracture toughness. The ductility is originated from easy slip of dislocations during deformation and fracture toughness is due to difficulty in nucleation of cracks and crack propagation and is related to stress concentration during deformation. The strength and ductility are strongly dependent on aging temperature and the size of alpha precipitation during aging is analysed and relationship between ductility and width of alpha phase is discussed and determined and the results show that the ductility of the alloy is higher than 6% when width of alpha is larger than 1micron.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

*Keywords: high-strength metastable beta titanium alloy, strength, fracture toughness, microstructure, aging*

# Mechanical properties and twinning-induced plasticity of metastable β-type Ti alloys

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## Abstract

Specific strength is one of the most important properties for biomedical and/or aerospace materials. In previous studies, various metastable β-type Ti alloys such as Ti-15V-3Al-3Cr-3Sn alloys were developed as a high strength Ti alloy. However, it is still necessary to improve the mechanical properties of the alloys, especially their ductility. Twinning-induced plasticity (TWIP) caused by {332}<113> deformation twinning is one of the effective mechanisms for improvement of the strength-elongation balance of the alloys.

In this study, deformation behaviours of metastable β-type Ti-Mo alloy which is primarily deformed by {332}<113> deformation twinning were studied by in-situ neutron diffraction measurements and deformation structure analyses. We directly observed for the first time that the α″ martensite phase is formed at the initial stage of the plastic deformation and the volume fraction of the phase increases with increasing deformation. Further increase in stress results in a replacement of the α″ phase by the {332}<113> twins. These results indicate that the stress-induced α″ martensite phase acts as a nucleation site for the {332}<113> twins. These findings contribute the development of a new alloy design method that can promote the deformation twinning. The newly metastable β-type Ti-Mn-Mo alloys designed with a focus on promoting TWIP exhibit not only good tensile properties but also excellent fatigue properties.

*Keywords: β-type Ti alloys, Mechanical properties, Twinning-induced plasticity, Neutron diffraction analysis*

# Microstructure evolution and strength-toughness of Ti2AlNb based alloy during across B2 forging

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**Abstract**

$Ti_2AlNb$-based alloy has excellent properties such as low density, high strength and high temperature resistance, and the application temperature can reach 650°C~750°C. It has the potential to replace the high density materials used at high temperature. It is an important candidate material for the preparation of aero-engine disk parts in the future. However, its practical application is restricted by the lack of effective matching of strength and toughness. In view of this problem, this work adopts across B2 forging technology to obtain bimodal size lamellar O phase microstructure, which can effectively improve the toughness of the alloy on the premise of ensuring the strength. During the forging process, the deformation dislocation in B2 phase has a significant influence on the precipitation behavior of subsequent O phase. At high strain rate, the interaction between the stress field of deformation dislocation and transformation strain of B2 phase into O phase lead to the strong variant selection of O phase, forming colony structure. At low strain rate, strong dynamic recovery occurs, and the anisotropy of dislocation stress field is significantly reduced. In this case, variant selection of O phase is weakened, and the basket-weave structure is formed. After solution and aging treatment, bimodal size lamellar O phase microstructure is obtained. The quasi-cleavage fracture is the main fracture mechanism of bimodal size lamellar O phase microstructure at room temperature. Cleavage of B2 phase dominates the fractures, and the cleavage cracks grow along the cleavage planes of B2 phase. The cleavage planes of B2 phase are measured to be {100} planes and {110} planes by trace method. Excellent microstructure can be obtained and adverse texture can be avoided through reasonable process control. The tensile strength of 1015MPa and fracture toughness of 49MPa·m1/2 are obtained under suitable process conditions.

*Keywords: $Ti_2AlNb$-based alloy, microstructure evolution, strength-toughness.*

# Technical **Oral Session _ Session 11**

## **Symposium E :** Additive Manufacturing

### Additive Manufacturing 11-1 (E11-1) — 10:50 -12:30, Nov. 23

**Chair :** Yoshitaka ADACHI (Nagoya University) — Halla Hall B, 3F

10:50-11:20 **K-E1160** **[Keynote] Friction stir based additive manufacturing technologies**
Fengchao Liu (Chinese Academy of Sceicne, Institute of Metal Research, China)

11:20-11:40 **I-E0300** **[Invited] Crystal plasticity analysis of plastic deformation behavior of AM structure with customized local texture**
Tsuyoshi MAYAMA (Kumamoto University, Japan)

11:40-12:00 **I-E1123** **[Invited] Deformation faulting and dislocation-cell refinement in a selective laser melted 316L stainless steel**
Feng He (Northwestern Polytechnical University, China)

12:00-12:15 **O-E1042** **Application of Laser Powder Bed Fusion in-situ alloying technology on medium entropy alloys**
Yaqing Hou (China Iron And Steel Research Insititute Group, China)

12:15-12:30 **O-E0660** **Characterization on Microstructure and Deformation Mechanisms of Selective Laser melted Ti-6Al-4V**
Yoon-Hwan Jo (Changwon National University, Korea)

# Friction stir based additive manufacturing technologies

**Fengchao Liu**[1], Dingrui Ni[2], Zongyi Ma[3]

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## Abstract

As an effective supplement to the traditional material preparation and processing methods, Additive Manufacturing technology is expected to meet the new demand for the short-cycle preparation of large-size and high-performance components in the field of advanced manufacturing. However, it is difficult to avoid solidification defects in the preparation of large components commercial non-weldable metals by fusion-based additive manufacturing technologies, which leads to the decline of the material mechanical properties of the fabricated components. The friction stir based solid-state additive manufacturing technologies were able to was avoid solidification defects, and fabricate dense, and fine grained component with weak texture, leading to improvement in the mechanical properties of the fabricate components. This paper reviewed the research progress and the application of friction stir based additive manufacturing technologies, and analyzed the challenges and trends in developing friction stir based additive manufacturing. The objective is to provide useful references for advancing the research in related fields.

*Keywords: Friction surfacing deposition additive manufacturing; Sheet-based friction stir additive manufacturing; Additive friction stir deposition; Additive friction extrusion-deposition; high-strength aluminum alloy.*

# Crystal plasticity analysis of plastic deformation behavior of AM structure with customized local texture

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## Abstract

Recently, novel crystallographic texture control technique was developed by using LPSB (laser powder bed fusion) additive manufacturing (AM) technology. This technique makes possible to fabricate single-crystal-like microstructure (SCM) where crystal orientations are strongly oriented. Furthermore, under appropriate process parameters, self-organized crystallographic lamellar microstructure (CLM) is also developed where main and sub layers have specific crystal orientations relative to building direction (BD) and scan direction. In this study, crystal plasticity analysis was performed to investigate possible mechanical properties of AM structure consisted of 2×2×2 blocks with SCM and/or CLM. Nickel based superalloy IN718 was assumed for a model material in the analysis where material parameters were identified based on the experimental stress-strain curves and deformed shapes. Numerical results indicated that self-organized lamella interfaces affected active deformation modes during plastic deformation. Finally, possible mechanical properties of AM structure were numerically explored. The results showed that yield stress and strain hardening behavior depend on the configuration of SCM and CLM blocks.

*Keywords: Finite element method, Crystal plasticity, Plastic deformation, Texture, Anisotropy*

# Deformation faulting and dislocation-cell refinement in a selective laser melted 316L stainless steel

Feng He[1], Chao Wang[1], Bin Han[2], Guma Yeli[3], Xin Lin[1], Zhijun Wang[1,*], Lilin Wang[1,*], Ji-jung Kai[4,*]

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## Abstract:

The selective laser melted (SLM) 316L stainless steel (316L SS) has shown superior tensile ductility and doubled yield strength compared to its wrought counterpart. The significantly improved yield strength has been attributed to the unique cellular substructures featured by Cr/Mo-segregation and trapped dislocations. The excellent ductility of SLMed 316L SS has been mainly understood from the pronounced deformation twinning, which, however, is just one of the dominant plastic deformation mechanisms in 316L SS. Here instead, we report two other fundamental deformation micro-mechanisms, i.e., deformation faulting and dislocation cell refinement, in the SLM 316L SS. Our results showed that deformation faulting and dislocation cell refinement characterize the whole tensile deformation significantly except for deformation twinning. These newly found mechanisms synergistically dominated the deformation behavior at low strain levels while deformation faulting and twinning play a crucial role at medium and high strain levels. The pre-existing stacking faults (SFs) in cellular substructure is mainly responsible for the significant deformation faulting. At the early deformation stage, these pre-existing SFs provide faulting nuclei for deformation faulting, leading to wide SFs. These wide SFs in different cellular interiors penetrate the cellular boundaries and overlap as the strain increases, resulting in long stacking fault ribbons (SFRs). We attributed the formation of DCs to the measured medium stacking fault energy (SFE) of ~18 mJ/m$^2$. Upon straining, equiaxed dislocation cells (DCs) were generated by new dislocation cell walls (DCWs) inside the cellular substructure, and refined by either the dissociation of fully developed DCWs or the continuously formed new DCWs. Together with deformation twinning, these two fundamental deformation mechanisms jointly led to a steady strain hardening rate during tension and thus a superior tensile ductility of the SLM 316L SS with high yield strength. These findings provide new insights into the excellent strength-ductility combination of SLMed 316L SS and the experimental basis for crystal plasticity modeling and simulation, as well.

**Keywords:** additive manufacturing, micro-mechanisms, deformation substructure, dislocation cell

# Application of Laser Powder Bed Fusion in-situ alloying technology on medium entropy alloys

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## Abstract

The Laser Powder Bed Fusion (LPBF) in-situ alloying is a novel technology for preparing novel alloys efficiently, which can overcome the problem of limited source of raw material powder. However, the narrow process window limits its application. A micro-scale integrated simulation model is designed and constructed based on the Discrete Element Method (DEM), the Finite Element Method (FEM), and Calculation of phase diagram (CALPHAD) method in the work. By defining the parameters such as composition inhomogeneity ω, the forming performance of LPBF in-situ alloying FeCoCrNi medium entropy alloys are predicted. The calculation results show that the hysteresis diffusion effect makes the mixing powders more challenging to be in-situ alloyed than conventional main component alloys. For the mixed powder beds consisting of 15-53 μm particles with equal mass ratio, laser remelting process are indispensable to eliminate unmelted elements, the composition inhomogeneity of as-printed samples can reach 98.7% by adding laser remelting processes for three times. High-efficiency preparation experiment of non-equiatomic ratio medium entropy alloy was carried out by using the technology. The tensile strength of in situ alloying samples are equivalent to that of the pre-alloyed powder samples under the optimized process conditions. The laser in-situ alloying parameters of FeCoCrNi alloy with equal atomic ratio is also suitable for non-equal atomic ratio alloys. The tensile property of non-equal atomic ratio alloys can be 20% higher than that of equi-atomic alloys.

*Keywords: High-throughput preparation; Laser powder bed fusion in-situ alloying; CALPHAD; Medium entropy alloy; Integrated calculation.*

# Characterization on Microstructure and Deformation Mechanisms of Selective Laser Melted Ti-6Al-4V

**Yoon-Hwan Jo[1],** Hyun-Uk Hong[2*], Chan-Hee Lee[3], Chiwon Kim[4], Jungmin Han[5], Yonghyuk Choi [6]

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## Abstract

Ti-6Al-4V alloy has been investigated for application in transportation industries, owing to its combination of high specific strength and toughness. For the efficient fabrication of components using Ti-6Al-4V alloy, the selective laser melting (SLM) process has been actively considered. As-built Ti-6Al-4V alloy consists of fine α' martensitic structure with prior columnar β grains due to high cooling rate during SLM process. The needle-like α' martensitic structure exhibits high strength, but inferior toughness because of its low ductility. To enhance the toughness of as-built Ti-6Al-4V alloy, proper post heat treatment has to be applied. In this study, to optimize the post heat treatment, various conditions were applied to the as-built Ti-6Al-4V alloy. The width of α+β lamellar increased with increasing temperature, while its hardness gradually decreased. After tensile test, Ti-6Al-4V alloy which was heat-treated at temperature near β transus (~995 ℃) exhibited improved elongation, showing ductile fracture. However, in the case of Ti-6Al-4V alloy which was heat-treated at lower temperature exhibited poor elongation, showing brittle fracture. From these results, it was confirmed that post heat treatment at high temperature near β transus is recommended for the optimization of post heat treatment condition in SLMed Ti-6Al-4V alloy. In this study, the optimum heat treatment design has been proposed, and discussed its effect on the characteristics of α+β lamellar structures in terms of α coarsening, β thickness, α+β lamellar width.

*Keywords: Ti-6Al-4V, Selective Laser Melting, Post heat treatment, Hardness, Tensile*

# Technical **Oral Session _ Session 11**

## **Symposium E :** Additive Manufacturing

**Additive Manufacturing 11-2 (E11-2)** **10:50 -12:45, Nov. 23**

Chair : Pan Wang (Singapore Institute Of Manufacturing Technology, A*STAR Research Entities) 303A, 3F

10:50-11:10 **I-E0562** **[Invited] Crystallographic texture formation and corrosion resistance of powder bed fusion-manufactured 316L stainless steel**
Takuya ISHIMOTO (University of Toyama, Japan)

11:10-11:25 **O-E0049** **Enhanced mechanical performance of duplex stainless steels via in-situ formation of core-shell nano-inclusions upon selective laser melting**
Haokai Dong (South China University Of Technology, China)

11:25-11:40 **O-E0176** **Transmission Electron Microscopy Studies on Orientation-Controlled 316L Austenitic Stainless Steel Produced by Laser Powder Bed Fusion**
Kazuhisa Sato (Osaka University, Japan)

11:40-11:55 **O-E0533** **Research on Microstructure and Mechanical Properties of Al-Mn-Mg-Sc-Zr-Hf Alloy Manufactured by Laser Powder Bed Fusion**
Qiuge Li (Northwestern Polytechnical University, China)

11:55-12:15 **I-E0657** **[Invited] Enhancing Additive Manufacturing through Core-Shell Composite Powders and in situ Dispersoid Synthesis for Metal Matrix Composites**
Ho Jin RYU (Korea Advanced Institute of Science and Technology, Korea)

12:15-12:30 **O-E0078** **Computational design of novel Ni superalloys with low crack susceptibility for additive manufacturing**
Hao Yu (Northeastern University, China)

12:30-12:45 **O-E0085** **The new Thermo-Calc Additive Manufacturing Module**
Johan Bratberg (Thermo-Calc Software, Sweden)

# Crystallographic texture formation and corrosion resistance of powder bed fusion-manufactured 316L stainless steel

**Takuya Ishimoto**[1]

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## Abstract

Metal additive manufacturing (AM) has been recognized in recent years as a methodology that enables to functionalize metallic materials by modification of the internal metallurgical microstructure, not only the shape of the product. We successfully developed wide range of crystallographic texture from a single crystalline-like to randomly oriented polycrystalline textures in a 316L stainless steel via laser powder bed fusion (LPBF). Worth noting, we developed a unique "crystallographic lamellar microstructure", in which two differently oriented grains appear alternately. This microstructure showed improved strength over those without the lamellar structure. Furthermore, the rapid cooling of LPBF significantly suppressed the formation and growth of inclusions that normally appear in 316L, resulting in a dramatic improvement in pitting corrosion resistance. This good corrosion resistance is almost independent of crystal orientation, i.e., exposed surfaces, which means that textures can be selected according to mechanical requirements without concern for corrosion resistance.

This work was supported by CREST-Nanomechanics (JPMJCR2194) from the Japan Science and Technology Agency, and Grant-in-Aid for Transformative Research Area (A) (JP21H05197).

*Keywords: Powder bed fusion, Crystallographic texture, Cooling rate, Localized corrosion*

# Enhanced mechanical performance of duplex stainless steels via in-situ formation of core-shell nano-inclusions upon selective laser melting

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## Abstract

Oxygen content with more than 20 ppm is normally recognized as a major issue in steels, as the formation of macro-scale oxide inclusions can significantly degrade the mechanical properties via weakening the metal/inclusion interface or promoting the large oxide cracking. Here we report a role exchange of oxides from detrimental to beneficial in a 2205 duplex stainless steel (DSS) fabricated by selective laser melting (SLM). With aid of minor Ti addition, substantial core-shell structured nano-inclusions with an oxide core and a TiN shell are obtained. Combined with high dislocation density, the unique as-built microstructure leads to an ultrahigh tensile strength (~ 1.2GPa) yet acceptable total elongation (~ 30%). Moreover, these nano-inclusions can also refine the microstructure by inhibiting the recrystallized grain growth and austenite formation upon the post-annealing treatment, and contribute to a notable precipitation strengthening increment up to ~230 MPa. The present nano-inclusions strengthened DSS exhibits an attractive mechanical performance with a tensile strength of ~910 MPa and a total elongation of ~52% yet non-deteriorative corrosion resistance, which has overwhelmed most of the reported 2205 DSSs. Our results provide a new route for developing a wide range of nano-architectured SLM alloys with drastically enhanced properties.

*Keywords: additive manufacturing; duplex stainless steel; core-shell structure; nano-inclusions; mechanical properties*

# Transmission Electron Microscopy Studies on Orientation-Controlled 316L Austenitic Stainless Steel Produced by Laser Powder Bed Fusion

**Kazuhisa Sato**[1], Shunya Takagi[1], Satoshi Ichikawa[1], Takuya Ishimoto[2,3,4], and Takayoshi Nakano[2,3]

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## Abstract

We have studied the microstructure and solute segregation around the melt-pool boundary of orientation-controlled 316L austenitic stainless steel produced by laser powder-bed fusion using transmission electron microscopy and energy-dispersive x-ray spectroscopy. We found that the solidification cellular microstructures were visualized with the aid of solute segregation (Cr and Mo) during solidification. Mn–Si–O inclusions (10–15-nm in diameter) were distributed along the lamellar boundaries, as well as in the dislocation cell walls. It is considered that grain growth of the inclusions can be effectively suppressed by rapid quenching during the laser powder-bed fusion process. The cellular spacing widened near the bottom of the melt-pool boundary owing to the decrease in the cooling rate. The low mobility of the solid/liquid interface will stabilize the planar solidification. In fact, a thin region without cellular microstructures was observed at the melt-pool boundary, possibly a planar solidification zone. Atomic-structure analysis at the lamellar boundary by high-resolution transmission electron microscopy revealed a local interfacial structure, which is complementary to the results of electron back-scatter diffraction [1].

[1] K. Sato, S. Takagi, S. Ichikawa, T. Ishimoto, T. Nakano, *Materials* **16** (2023) 218.

This study was supported by Grant-in-Aid for Transformative Research Area (A) (Grant No. 21H05196) from the MEXT, Japan.

*Keywords: additive manufacturing; laser powder-bed fusion; cellular microstructure; solidification segregation; transmission electron microscopy*

# Research on Microstructure and Mechanical Properties of Al-Mn-Mg-Sc-Zr-Hf Alloy Manufactured by Laser Powder Bed Fusion

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## Abstract:

Laser Powder Bed Fusion (L-PBF), as an advanced metal additive manufacturing technology, which enables a non-equilibrium microstructure with a supersaturated metal matrix, coherent/semi-coherent metastable phases, and high dislocation densities, contributes to the advanced mechanical performance required for modern engineering applications. Aluminum alloys have attracted much attention due to their combination of corrosion resistance, high specific strength, good thermal/electrical conductivity, hence being regarded as one of the most promising lightweight and high-strength structural materials for aerospace applications. In this work, a new high-strength Al-Mn-Mg-Sc-Zr-Hf alloy with excellent L-PBF printability was developed and prepared. The microstructure evolution mechanism and mechanical properties were investigated and the synergistic effects of various strengthening mechanisms of the L-PBFed samples were clarified.

The Al-Mn-Mg-Sc-Zr-Hf alloy prepared by L-PBF at the as-built state has a multi-scale grain size distribution with heterogeneous microstructure in which micron-sized coarse columnar grain (with an average grain size of 2.94 ±1.6 μm) and medium equiaxed grain (with an average grain size of 1.64 ± 0.39 μm) are generated in the center of the melt pool, while submicron-sized ultrafine equiaxed grain (with an average grain size of 0.63 ± 0.07 μm) appears at the edge. The second phase particles are inhomogeneously distributed in different regions of the melt pool. Specifically, the cuboid primary Al3(Sc,Zr,Hf) mainly shows in the ultrafine equiaxed grain region, and Al6Mn precipitates along the grain boundaries in the coarse columnar grain regions in spherical while irregular-shaped in the ultrafine equiaxed grain region. The presence of Al12Mg17 indicates slight microsegregation occurred at the grain boundaries.

The L-PBFed Al-Mn-Mg-Sc-Zr-Hf alloy samples along the horizontal direction exhibit a favorable combination of strength and plasticity, with 538 ± 1 MPa in tensile strength, 496 ± 5 MPa in yield strength, and 10 ± 1% elongation. While the tensile strength, yield strength, and elongation along the vertical orientation are 498 ± 1 MPa, 439 ± 1 MPa, and elongation 6 ± 1%, respectively, signifying a distinct anisotropy at the as-built state. In addition, the fracture morphology of the L-PBFed Al-Mn-Mg-Sc-Zr-Hf tensile samples at the as-built state shows the characteristics of brittle fracture. The cracks in the coarse columnar grain region expand but are effectively suppressed in the ultrafine equiaxed grain region.

*Keywords:Additive Manufacturing; Laser Powder Bed Fusion; High-strength Aluminium; Alloy Design; Strengthening Mechanisms*

# Enhancing Additive Manufacturing through Core-Shell Composite Powders and in situ Dispersoid Synthesis for Metal Matrix Composites

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## Abstract

Challenges remain in preparing feedstock powder and operating the additive manufacturing process of metal matrix composites. This study addresses these issues by introducing a novel Surface Modification and Reinforcement Transplantation (SMART) process, featuring a metal core and composite shell. Inconel 625/TiCp composites fabricated with this powder technique exhibit improved strength and reduced defects, offering superior properties and reliability through high dislocation density and reinforcement dispersion, surpassing traditional casting and powder metallurgy techniques. Additionally, additive manufacturing of wrought aluminum alloys has encountered obstacles due to unfavorable characteristics. Incorporating $B_4C$ reinforcement in a novel core-shell powder ensured stable metal additive manufacturing behavior for aluminum matrix composites. Directed energy deposition with the $B_4Cp$/6061 MMC powder mitigated cracks, pores, and balling while refining grain structure and enhancing mechanical properties. Moreover, the study introduces a novel approach for oxide dispersion-strengthened alloys in additive manufacturing. Employing in situ dispersoid synthesis through $TiO_2$ addition yields reduced dispersoid size and strengthens the CoCrNi MEA matrix. This research highlights the potential of fabricating ODS alloys with optimal microstructures using DED and in situ dispersoid synthesis facilitated by Ti and O suppliers. This research highlights the potential of additive manufacturing for fabricating metal matrix composites with tailored properties and improved performance by introducing novel core-shell composite powders via an innovative SMART process.

*Keywords: Additive manufacturing, metal matrix composites, core-shell composite powder, in situ dispersoid synthesis*

# Computational design of novel Ni superalloys with low crack susceptibility for additive manufacturing

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## Abstract

Additive manufacturing (AM) has enabled the fabrication of innovative, geometrically complex components of metallic materials with minimal material waste. However, the application of AM in processing Ni superalloys remains challenging due to the high crack susceptibility. To address this problem, a computationally design method was applied to design novel Ni superalloys with low crack proneness as well as decent service performance. Different types of crack formation mechanisms during AM processing, i.e., the hot tear cracks and the strain-age cracks, have been taken into account, while a series of corresponding criteria to quantitively describe the crack susceptibility were parallelly analyzed. To select the most proper criteria as optimization index in alloy design regime, a series of prototype alloys with wide range of alloying elements were printed, with their crack behaviors being quantitively captured. The Freezing Range criterion and Stain Age Crack criterion were then determined as the optimization index in the design routine. A genetic algorithm was applied to probe the compositional search domain, while a Pareto front linking the hot tear crack criterion and strain age crack criterion was constructed by combining results of two separate optimization routes. Novel Ni compositions with optimized crack resistance as well as decent microstructural features were thereby identified. The new solutions are predicted to possess fairly better crack formation resistance compared to existing Ni superalloys. Moreover, the newly designed alloys manage to computationally outperform the existing printable alloys in all aspects of temperature capability, creep properties and oxidation resistance.

*Keywords: Additive manufacturing, Ni superalloys, Computational design, Thermodynamics and kinetics*

# The new Thermo-Calc Additive Manufacturing Module

Johan Bratberg, Amer Malik, Quang Minh Do, Johan Jeppsson

Today's state-of-the-art Finite Element (FEM) tools tend to use relatively simplified materials descriptions using handbook values that might have little dependence on chemistry or even temperature. Thermo-Calc has spent the last few years developing new models to predict thermophysical material properties to incorporate with CALPHAD-based materials descriptions. This is currently used to extract CALPHAD-based materials data for use in dedicated FEM codes and is now laying the foundation for our development of a completely integrated tool to simulate Additive Manufacturing (AM) processes. The AM Calculator is released in Thermo-Calc version 2023b, and it gives a unique possibility to address the problem of solidification during AM, where we obtain a unified treatment of both process parameters and chemistry-dependent thermophysical properties when solving the multi-physics problem of a moving heat source that melts and solidifies metal powder. The updated Scheil calculator allows for pre-generating a solidification profile, now also including evaporation properties, that can be saved into your own materials library, or used directly as input to the AM Calculator. Examples of the AM module applied to different material classes are shown.



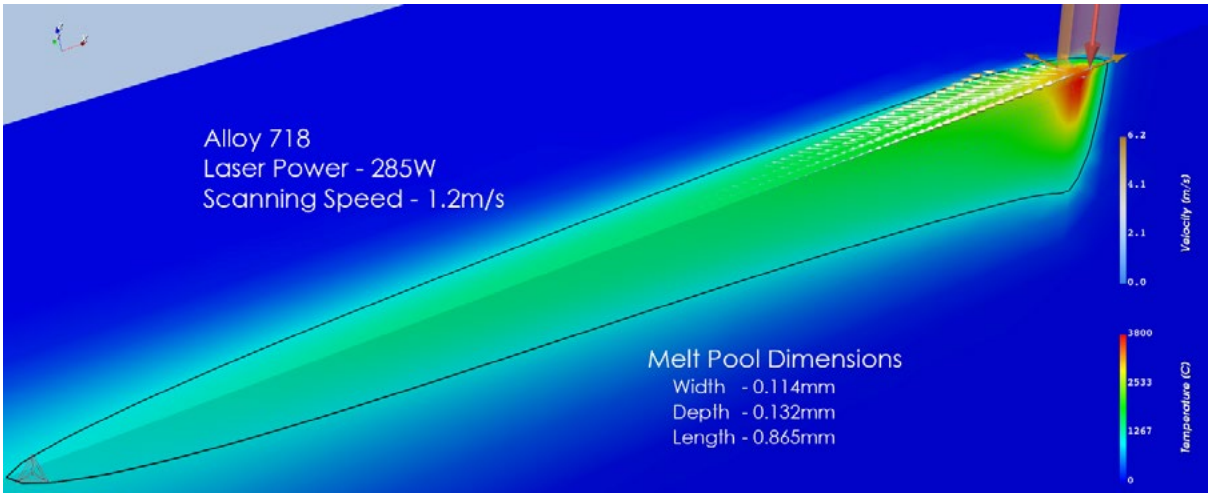



Fig.1. Steady state simulation of alloy 718 using the below calculated Thermophysical properties calculated using Scheil with freeze in model for a specific 718 chemistry.

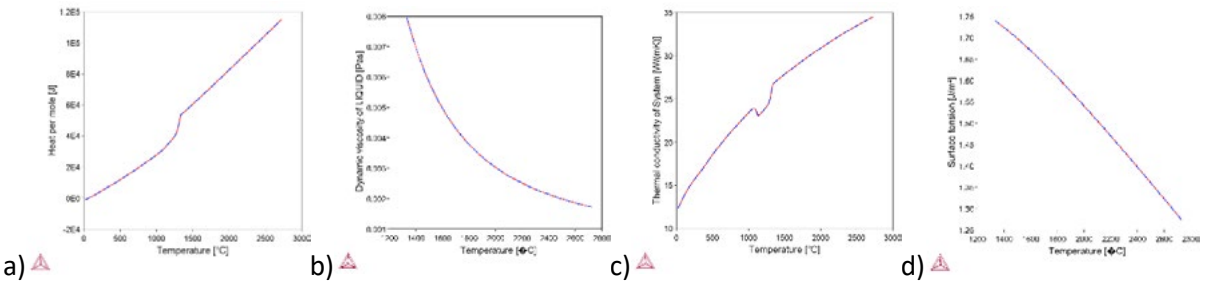



Fig. 2 a-d. (a) Heat per Mole vs Temperature, (b) Viscosity vs Temperature, (c) Thermal Conductivity vs Temperature and (d) Surface Tension of Liquid vs Temperature

# Technical **Oral Session _ Session 11**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 11 (K11)** **10:50 - 12:35, Nov. 23**

**Chair :** Kefu YAO (Tsinghua University) Samda Hall B, 3F

10:50-11:05 **O-K0148** **Cryogenic mechanical properties and deformation-induced FCC-HCP phase transformation of the precipitation-hardened metastable high-entropy alloys**
Jinseob Kim (Hanyang University, Korea)

11:05-11:20 **O-K0161** **Alloying Effect on the High Temperature Mechanical Property in Single Phase L12-ordered Intermetallic Alloys**
Chenyuan Wang (The University of Tokyo, Japan)

11:20-11:35 **O-K0151** **Co-precipitation of coherent and incoherent L12 particles to tailor the mechanical properties of a multico**
Guanghui Yang (Hanyang University, Korea)

11:35-11:50 **O-K0993** **Effect of hydrogen on mechanical behavior of as-cast and single crystal CoCrFeMnNi High-entropy alloy**
Hong Zhong (Northwestern Polytechnical University, China)

11:50-12:05 **O-K0607** **Development of novel Co-Ni-Fe eutectic high entropy alloy for a wide temperature application**
Kannan Ravi Ramkumar (Pohang University of Science and Technology, Korea)

12:05-12:20 **O-K0106** **Microstructure evolution and high-temperature mechanical properties of HCP-TiZrHf-high entropy alloys (HEAs)**
Shaoji Liang (The University of Tokyo, Japan)

12:20-12:35 **O-K0299** **Improvement in Mechanical Property of CoCuNi Medium Entropy Alloy by High-Pressure Torsion**
Sangmin Lee (National Institute for Materials Science, Japan)

# Cryogenic mechanical properties and deformation-induced FCC-HCP phase transformation of the precipitation-hardened metastable high-entropy alloys

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Topic area: High-Entropy Materials and Amorphous Materials

## Abstract

The precipitation-hardened metastable high entropy alloy containing carbon and microalloying elements showed excellent strength and ductility at room temperature by activation of various deformation mechanisms. Furthermore, previous research on metastable high entropy alloys reported better strength-ductility combination with decreasing deformation temperature from room temperature. Thus, we investigated temperature-dependent mechanical properties and deformation mechanisms of the $Fe_{50.15}Mn_{29.6}Co_{10.5}Cr_{9.3}Ti_{0.1}V_{0.1}Mo_{0.2}C_{0.05}$ (Wt.%). The investigated material was annealed at 700 ℃ for 1 h, and the microstructure showed the partially recrystallized FCC single phase containing precipitates such as $M_{23}C_6$ carbide, sigma, and Ti-rich carbide. Tensile tests were conducted at room temperature, 100°C, -50, -100°C, and -150°C. With decreasing deformation temperatures, strength continuously increases and ductility tends to decrease. However, in the deformation temperature range from -50°C to -150 °C, ductility loss was not observed. The amount of deformation-induced FCC to HCP transformation tends to increase with decreasing deformation temperatures but was similar in the deformation temperature range from -50°C to -150 °C. The EBSD kernel average misorientation maps of the deformed specimens showed an increase in local strain in both FCC and HCP phases with decreasing deformation temperatures, suggesting high plastic deformation accommodation in materials deformed at low temperatures. With decreasing deformation temperatures, back stress strengthening and multi-variant HCP plates increases. Detailed discussion on deformation mechanisms and mechanical properties will be presented.

*Keywords: High entropy alloy, Precipitation strengthening, Cryogenic mechanical properties, deformation mechanisms, Back stress*

# Alloying Effect on the High Temperature Mechanical Property in Single Ph: $L1_2$-ordered Intermetallic Alloys

**Chen-yuan Wang[1]**, Sae Matsunaga[2], Victoria A. Tucker[3], Hideyuki Murakami[4], An-Chou Ye Michael. S. Titus[6], Yoko Yamabe-Mitarai[7]

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## Abstract

γ'($L1_2$)-strengthened superalloys have been employed as high temperature structural materials d their excellent high temperature properties. In these alloys, it is well known that the dom deformation mechanism is γ' shearing events associated with the formation of planar defe intermediate temperatures, then it transfers to thermally-activated cross slip as temperature incre Recent works of the deformation at intermediate temperatures revealed that the segregation of sp alloying elements either assists the formation of planar defects or promotes aggressive microtwin It has been reported that the intense segregation of Co and Cr at the faults produced microtwi decreasing the energy barriers to remove wrong nearest-neighbor bonds along the faults, whil segregation of Ti, Ta, or Nb assisted in the formation of stable η or χ phases along the faults, resu in the significant improvement of creep resistance (Local Phase Transformation Strengthening). Furthermore, it was suggested that the small difference in nominal alloy compositions would act different deformation mechanisms. While the deformation at intermediate temperatures has actively conducted, the alloying effects on the increase of CRSS and activation of cross-slips ar not well understood. In order to further understand the correlation between the composition of γ' p and activated deformation mechanisms, we designed compositionally-complex single γ' phase a and performed high temperature mechanical tests in a wide range of temperatures. Our recent re of mechanical tests and high-resolution electron microscopy will be presented. Possible mechar behind the significant differences in mechanical responses will be discussed.

*Keywords: Composition complexity, , γ'-$Ni_3Al$, high temperature mechanical testing, Ni-based superalloys*

# Co-precipitation of coherent and incoherent $L1_2$ particles to tailor the mechanical properties of a multicomponent alloy

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Topic area: High-Entropy Materials and Amorphous Materials

## Abstract

$L1_2$-strengthened multicomponent alloys (MCAs) have recently received great attention owing to their promising mechanical properties. However, precipitation strengthening solely by "soft" coherent $L1_2$ particles is often not enough to achieve ultra-high strength. Here, we report a novel method to enhance precipitation strengthening in $Fe_{45.2}Ni_{30.1}Cr_{17.9}Al_{3.5}Ti_{3.2}$ MCA by introducing coherent and incoherent $L1_2$ particles. The material containing co-precipitated coherent and incoherent $L1_2$ particles shows a larger strength-ductility balance than the material only containing coherent $L1_2$ particles. Nanoindentation results showed that the nanohardness at the interior of grains containing co-precipitated coherent and incoherent $L1_2$ particles was slightly higher than that at grain boundaries, suggesting a strong strengthening effect of the incoherent $L1_2$ particles. Coherent and incoherent $L1_2$ particles were characterized by Transmission electron microscopy analysis in detail. The formation mechanisms of incoherent $L1_2$ particles and their role in mechanical properties will be discussed.

*Keywords: Multicomponent alloy, precipitation strengthening, $L1_2$ structure, nanohardness, mechanical properties*

# Effect of hydrogen on mechanical behavior of as-cast and single crystal CoCrFeMnNi High-entropy alloy

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## Abstract

High entropy alloy (HEA) has excellent mechanical properties, corrosion resistance and radiation resistance due to its unique alloy design concept and four effects. In the future, structural components made from high entropy alloys may be exposed to hydrogen in many potential working environments, such as ambient hydrogen in aerospace structures, high hydrogen content in water reactor environments in nuclear power plants, and hydrogen transport stored in high-pressure vessels.

Here, we prepared CoCrFeMnNi high entropy alloys with four different microstructures (as-cast polycrystal, dendritic single crystal, heat treated dendritic single crystal, directionally solidified polycrystal) by Bridgman directional solidification and heat treatment. Then the effect of hydrogen on the mechanical behaviour of high entropy alloys with various microstructures were studied.

Tensile fracture show that brittle layers appeared on the surface of as-cast samples subjected to electrolytic hydrogen charging, and the thickness of the brittle layer is strongly correlated with the hydrogen charging time. However, the fracture morphology of directionally solidified and single crystal samples is not significantly affected by hydrogen charging time. The results are related to the capture effect of grain boundaries on hydrogen.

*Keywords: High entropy alloy, Single crystal, Mechanical properties, Hydrogen embrittlement*

# Development of novel Co-Ni-Fe eutectic high entropy alloy for a wide temperature application

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## Abstract

A novel Co-Ni-Fe-based eutectic high entropy alloy (EHEA) has been developed by prefixing valance electron concentration (VEC), based on the requirement to balance strength and ductility in high entropy alloys (HEAs). The developed EHEA includes two-phase structures: the FCC phase and the ordered B2 phase as well as the ordered B2 precipitates. The developed HEA showed excellent mechanical properties in a wide range of temperatures (77 K, 298 K, 473 K, and 673 K). The strength and ductility become compromised at 473 K, i.e., yield strength 365 MPa, ultimate strength 826 MPa with 60% ductility. The phase transformation and deformation twins were absent during tensile loading. The dislocation motion in the soft FCC phase and their piling up at the FCC/B2 interface balanced the strength and ductility.

***Keywords:*** *Eutectic alloy; Dual phase; valance electron concentration; B2 phase; Strain hardening;*

# Microstructure evolution and high-temperature mechanical properties of HCP-TiZrHf-high entropy alloys (HEAs)

**Shaoji Liang[1]**, Sae Matsunaga [1], Yoko Yamabe-Mitarai[1]

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## Abstract

High-temperature (HT)-titanium alloys are widely used for fan blades and compressor components of aircraft jet engines. However, their high-temperature mechanical properties significantly deteriorate in the operating temperature exceeding 600℃. Further increasing the operating temperature of HT-titanium alloys will enable us to replace Ni-based superalloys with them, thereby decreasing the overall weight of aircraft engines. Recently, high entropy alloys (HEAs), composed of multiple elements in nearly equiatomic proportions have been attracting much attention, due to their superior characteristics such as higher strength than conventional alloys. The current state-of-art HT titanium alloys have the α-HCP phase as the primary phase, so we introduce the HEA concept to strengthen the primary HCP phase to improve high-temperature mechanical properties. However, investigating the HEA effect is challenging because it is generally impossible to separate the strengthening effect from (1) solid solution and (2) martensitic structure, which is the typical structure of commercial HT-titanium alloys. This study aims to investigate the high-temperature deformation mechanism of the equiaxed HCP-HEAs and evaluate their high-temperature mechanical properties to exclude the strengthening effect from a martensitic structure. Three alloys TiZrHf, TiZrHfAl, and TiZrHfAlSc were designed and fabricated based on thermodynamic calculations and prior knowledge about the alloying effect for phase stabilization. All alloys were hot-rolled and homogenized to promote the strain-induced formation of equiaxed grains. Our recent results of microstructure characterization and high-temperature mechanical tests will be presented. The compression deformation mechanism at room temperature and 600℃ will be discussed.

*Keywords: high entropy alloys, equiaxed-hcp phase, high-temperature compression strength, deformation mechanism.*

# Improvement in Mechanical Property of CoCuNi Medium Entropy Alloy by High-Pressure Torsion

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## Abstract

High/medium entropy alloys (H/MEAs) have been attracting much attention as a new class of metallic materials. In this study, the effect of high-pressure torsion (HPT) and post-HPT annealing on the microstructures and mechanical properties was studied for an equiatomic CoCuNi MEA.

The sample homogenized at 1423 K was in a FCC single phase. The as-homogenized (AH) specimen exhibited tensile strength of 400 MPa and 10% total elongation. After HPT deformation of 10 anvil rotations, the grain size was reduced to 90 nm, and the tensile strength and total elongation improved to 1.5 GPa and 16%, respectively. SEM observations of the fracture surfaces revealed that the fracture mode changed from brittle intergranular fracture to ductile fracture by HPT. 3D atom probe tomography (APT) unveiled heavy grain boundary segregation of Cu in the AH sample and removal of the segregation by the HPT deformation, which may explain the fracture mode change and improved ductility.

After the post-HPT annealing at temperatures above 873 K, the single FCC phase was decomposed into Cu-rich FCC and Co-Ni FCC phases concomitantly with the recrystallization. The compositions of the two FCC phases were close to those of the equilibrium estimated by the Calphad calculation. Tensile elongation increased with the expense of tensile strength by the post-HPT annealing. Boundary misorientation analysis by EBSD revealed that the number fraction of twin boundaries significantly decreased by the tensile deformation, suggesting that the observed increase in the elongation is partially due to the detwinning of the annealing twins.

*Keywords: CoCuNi medium entropy alloy (MEA), high-pressure torsion (HPT),3D atom probe tomography, mechanical property, segregation,*

# Technical **Oral Session**

Keynote, Invited and Contributed Oral Talk

## Session 12

November 23

14:00-15:30

# Technical **Oral Session _ Session 12**

## **Symposium A :** Advanced Steels and Properties

**Advanced Steels and Properties 12 (A12)** **14:00 – 15:30, Nov. 23**

**Chair :** Jeongho Han (Hanyang University) Halla Hall A, 3F

14:00-14:15 **O-A0019** **Microstructures and mechanical properties of a Ti-microalloyed High-strength steel subjected to quenching-tempering process**
Fanzheng Bu (TKAS Auto Steel Company Limited, China)

14:15-14:30 **O-A0033** **Effect of Heat Treatment on Microstructure and Properties of Hot Rolled Mn-Cu Based Damping Alloy**
Yao Huang (Harbin Engineering University, China)

14:30-14:45 **O-A0150** **Quenching and partitioning in a Si/Al-free steel realized by Mn patterning**
Zhiping Xiong (Beijing Institute of Technology, China)

14:45-15:00 **O-A0172** **Engineering chemical heterogeneity via fast heating to achieve strong yet ductile medium Mn steels**
Yan Wang (Tsinghua University, China)

15:00-15:15 **O-A0209** **Effect of Post-Heat Treatment on Microstructure and Mechanical Properties of 5% Cr Cold Work Tool Steel Manufactured Via Laser Direct Energy Deposition**
Jung-Hyun Park(Inha University, Korea)

15:15-15:30 **O-A1166** **Visualization of welding microstructure of high-strength bainitic steel and its relationship with ductile-brittle transition temperature (DBTT)**
Xuelin Wang (University of Science and Technology Beijing, China)

# Microstructures and mechanical properties of a Ti-microalloyed High-strength steel subjected to quenching-tempering process

**Fanzheng Bu[1]**, Qiang Guo[2], Qingmei Wu[3], Jingjiang Xiao[4], Xudong Sun[5]

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## Abstract

The influence of reheat quench and tempering on structure-property of Ti-Nb-Mo microalloyed steel was studied. The hot rolled steels were heat-treated by conventional reheat quenching and tempering technique, which introduced microstructural variation. This has resulted in ameliorative tempering of the as-quenched bainitic matrix, accompanied by nanoscale precipitation of Ti-riched carbides that highly dispersed in the matrix randomly. The microstructural characteristics, including detailed structure of microstructural constituents and precipitation behavior, as well as their effect on the yield strength and low temperature toughness were investigated. The results indicate that the yield strength and low temperature toughness showed significant improvement after quenching and tempering, which is much superior to that of hot rolled steel. TEM observation revealed that the precipitation characteristics were similar in both hot rolled and reheat quenching steel but slightly larger for the latter in terms of size. Whereas, in as-tempered steel, most of nanoscale carbides precipitated finely and densely in the tempering stage and thus highly contributed to the increase of the strength accompanied by bainite transformation. TEM studies are made with a view to understanding and correlating the mechanical properties with the microstructures, which indicate that the higher fraction of bainitic microstructure with the presence of lath-type bainitic ferrite and tiny polygonal ferrite is thought to be responsible for the improvement of low temperature impact toughness.

*Keywords: Microalloyed steels; tempering and quenching; microstructural characterization; precipitation; mechanical properties*

# Effect of Heat Treatment on Microstructure and Properties of Hot Rolled Mn-Cu Based Damping Alloy

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## Abstract

For Mn-Cu based damping alloys, when aging treatment is performed in the miscibility gap, the alloy will undergo spinodal decomposition, forming a certain manganese rich region, promoting martensitic transformation, and improving its damping performance. In this paper, Mn-23.65Cu-5.13Ni-2Fe-2Zn-0.05Ce (wt.%) damping alloy with a hot rolling deformation of 80% was prepared and subjected to solution treatment. On this basis, the effects of different aging temperatures and holding times on the properties of hot-rolled Mn-Cu damping alloys were studied. The Martensitic transformation twins and α-Mn precipitated phase were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD). Combined with lattice distortion, the variation of microstructure and phase structure of Mn-Cu based damping alloy were analyzed in detail. Then, the damping properties, room temperature tensile properties, and tensile fracture morphology of the Mn-Cu based damping alloy were further characterized and analyzed to obtain a more suitable heat treatment process. The results show that the damping properties of Mn-Cu based damping alloys show a trend of first increasing and then decreasing with the increase of aging temperature and holding time. The hardness, yield strength, and tensile strength of the alloys gradually increase, while the elongation after fracture gradually decreases. This shows, after aging at 430 ℃ for 7 hours, the Mn-Cu damping alloy has good comprehensive properties.

*Keywords: Mn-Cu based damping alloy; Hot rolling deformation; Damping performance; mechanical property*

# Quenching and partitioning in a Si/Al-free steel realized by Mn patterning

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## Abstract

Carbon partitioning is the feasible way to stabilize austenite against martensite transformation at room temperature in quenching and partitioning (Q&P) steels and thus, Si/Al addition is necessary to inhibit competitive reactions like carbide precipitation. Here, we realize carbon partitioning from martensite to austenite in a Si/Al-free Q&P steel. In the quenching step, Mn-enriched austenite and Mn-depleted martensite are obtained through fast heating and short austenitization from initial Mn-partitioned pearlite, which consists of Mn-enriched cementite and Mn-depleted ferrite. This is called Mn patterning. Followed by partitioning, carbide precipitation is wholly prevented, making carbon diffuse from martensite to austenite. This phenomenon is directly evidenced by atom probe tomography. The absence of carbides in the martensite is striking; it is probably ascribed to the Mn enriched in austenite, which has a strong attraction with carbon. Increasing quenching temperature from 60 to 110 °C increases the width of retained austenite from 43.8±11.8 to 47.7±9.7 nm and its fraction from 18.7 % to 23.2 %. All the fractions and widths of retained austenite in Q&P process are larger than those (33.6±6.4 nm; 11.2%) after directly quenching from austenitization to room temperature. Additionally, the tensile properties are comparable with conventional Q&P steels having similar carbon content of 4 wt. %, showing 2000 MPa tensile strength and 14.4 % total elongation. It is convinced that this work offers a novel avenue to produce Q&P steels without Si/Al addition through Mn patterning between austenite and martensite.

*Keywords: carbides; quenching & partitioning; silicon; retained austenite.*

# Engineering chemical heterogeneity via fast heating to achieve strong yet ductile medium Mn steels

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**Abstract**

Excellent combination of strength and ductility has made medium Mn steels (MMS) one of the most promising candidates of Advanced High Strength Steels (AHSSs). While work hardening ability of MMS can be substantially improved by metastable austenite, the relative soft ferrite matrix makes it hard to achieve a high yield strength in MMS. In the present study, chemical heterogeneity concept and fast heating technology were successfully employed to architecture a novel duplex microstructure consisting of ultrastrong martensite matrix and metastable austenite in MMS. Austenite stability and fraction are carefully designed by adjusting Mn and C distribution, resulting in varied transformation induced plasticity (TRIP) effect. By engineering chemical heterogeneity, excellent mechanical properties of total elongation (~20%) and ultimate strength (~1600MPa) were achieved in an Fe-0.22C-4Mn-0.4Si-0.05Nb-0.05Mo steel. Combining fast heating and chemical heterogeneity concept is expected to be an effective strategy to architecture novel microstructures and unique mechanical properties in other AHSSs.

*Keywords: Medium Mn steels, Chemical heterogeneity, TRIP, Retained austenite, Flash heating*

# Effect of Post-Heat Treatment on Microstructure and Mechanical Properties of 5% Cr Cold Work Tool Steel Manufactured Via Laser Direct Energy Deposition

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## Abstract

5 wt.% chromium tool steel exhibits high mechanical properties and crack resistance, which are derived from its martensitic structure and controlled alloying elements that result in fine carbide precipitation. In this study, crack-free 5 wt% Cr cold work tool steel with high-density was fabricated by the direct energy deposition (DED) process for the first time. The manufactured specimens were subjected to post-heat treatment composed of austenitizing and tempering. The initial microstructural characteristics before and after post-heat treatment were analyzed, and mechanical properties were evaluated using hardness, tensile, and compression tests. The initial microstructure was mainly composed of martensite and austenite boundary regions, with a carbide network formed along the build direction. The carbide network consisted of block-type and lamellar-type carbides rich in Cr, Mo, and V, with polygonal ferrite formed around them. After post-heat treatment, the microstructure transformed to acicular martensite, and the carbide network was separated into fine block-type carbides. The Vickers hardness measurement results showed a value of 710.2 ± 11.0 HV in the as-built state, and 649.1 ± 9.3 HV after post-heat treatment. The average ultimate tensile strength increased from 1340.4 ± 17.0 MPa to 1949.4 ± 28.2 MPa, yield strength increased from 779.5 ± 14.3 MPa to 1299.5 ± 15.9 MPa, and elongation decreased from 1.1% to 0.7% after post-heat treatment. Additionally, the compressive yield strength increased from 2147.2 ± 31.1 MPa to 2312.7 ± 60.5 MPa, showing superior hardness-compressive yield strength combination compared to other high-strength steel manufactured by additive manufacturing. Based on the above results, the deformation mechanism of 5 wt.% chromium tool steel manufactured by DED was also discussed.

*Keywords: Direct energy deposition, 5 wt% Cr cold work tool steel, post-heat treatment, microstructure, mechanical property*

**Symposium: Advanced Steels and Properties**

# Visualization of welding microstructure of high-strength bainitic steel and its relationship with ductile-brittle transition temperature (DBTT)

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## Abstract

Engineering structural steels such as wind power steel and offshore steel have achieved excellent comprehensive properties of high strength, high toughness, and high plasticity due to the use of low-carbon bainite structure control technology, and are widely used in major engineering construction. However, with the increase of strength and the improvement of environment requirements, the key performance and service safety issues of engineering components are highlighted in welded joints. The selection of welding materials and the matching of welding processes have become key decisive factors in determining the microstructure and properties of the weld metal (WM) and heat affected zone (HAZ). In this study, microstructure and ductile-brittle transition temperature (DBTT) evolution in welded zone obtained by using submerged arc welding (SAW) and laser hybrid welding (LHW) were elucidated from the aspect of crystallographic structure, particularly, digitization and visualization of 24 variants. The impact toughness of each micro zone in LHW joint is better than that of SAW, in which the DBTT of equivalent fusion line and HAZ can reach -70 and -80 °C, while that of SAW is only -50 °C, correlating with the variant selection mechanism of bainitic transformation. In addition, in order to ensure the performance of HAZ and avoid austenite grain coarsening, the effects of different initial microstructures on the reverse austenite nucleation and grain refinement during reheating were studied. It is found that lath bainite (LB) is more conducive to refinement of austenite grain and transformation structure after welding or heat treatment.

*Keywords: Bainitic steel, welding, lath bainite, variant selection, reverse transformation*

# Technical **Oral Session _ Session 12**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 12-1 (D12-1)** **14:00 -15:20, Nov. 23**

**Chair :** Jae Yeon Kim (Korea Institute of Materials Science) Samda Hall A, 3F

14:00-14:20 **I-D0789** **[Invited] Research on the microstructure and properties of ultralight Mg-Li-X Alloys**
Yan Yang (Chongqing University, China)

14:20-14:35 **O-D0162** **Effect of cooling rate on corrosion behavior of Mg alloy containing high Al**
HONGXIU LIU (Korea Institute of Materials Science, Korea)

14:35-14:50 **O-D0750** **Tribocorrosion behavior of Mg alloys in Hank's solution**
Eri Miura-Fujiwara (University of Hyogo, Japan)

14:50-15:05 **O-D0699** **Effect of microstructure on tensile properties of Mg-Al-Zn alloy in humid air**
Toshiaki Manaka (National Institute Of Technology(KOSEN), Niihama, USA)

15:05-15:20 **O-D0143** **The influence of mischmetal (Ce, La) on the corrosion properties of AZ91 - Ca - Y alloy**
Wen Ding (Korea Institute of Materials Science, Korea)

# Research on the microstructure and properties of ultralight Mg-Li-X Alloys

Yan Yang, Gang Zhou, Xiaodong Peng, Fusheng Pan

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**Abstracts:**

The engineering application of ultra-light Mg-Li alloys is seriously restricted because of their low strength, poor stability and high temperature performance. Ultralight Mg-Li-X alloys with high strength were designed and prepared via the introduction of alloying element and plastic deformation. Ultralight Mg-Li-Al-Sn, Mg-Li-Al-Mn and Mg-Li-Al-Ca alloys with high strength and good damping capacities have been developed in our research group. The microstructure, mechanical properties and damping property of Mg-Li-Al-X alloys were investigated systematically combing the usage of many advanced microstructure characterization methods and normal tensile tests, etc. The results from this research provide important technological support for the controlling of microstructure, mechanical properties and damping capacities of Mg-Li alloys.

**Keywords:** Mg-Li alloys, Plastic deformation, Microstructure, Mechanical properties, Damping capacity.

# Effect of cooling rate on corrosion behavior of Mg alloy containing high Al

**Hongxiu Liu**[1], Jun Ho Bae[2], Wen Ding[3], Jun Seob Lee[4], Bong Sun You[5*]

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## Abstract

The cooling rate has a significant influence on the microstructure and mechanical properties of Mg alloy, which has been widely studied. Additionally, it has been reported that the cooling rate also affects the corrosion properties of Mg alloy. As we all know, mechanical properties such as hardness and tensile strength can be greatly improved by increasing the Al content. However, the relationship between Al content and corrosion properties is still unclear. Based on our previous research, Ca and Y have been shown to have a positive effect on corrosion resistance. Therefore, this study investigates the effect of cooling rate on the corrosion behavior of Mg alloy containing Zn, Mn, Ca, Y, and varying Al contents (9, 11, and 13 wt%).

*Keywords: Mg alloy, High Al content, Cooling rate, Corrosion behavior.*

# Tribocorrosion behavior of Mg alloys in Hank's solution

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## Abstract

Tribocorrosion behaviors of AZ31 and WE43 were investigated during the sliding wear test in Hank's balanced salt solution (HBSS) and pure water. Wear volume variation against dead load from 0.98 N to 5.88 N shows that the wear volume increased monotonically with increasing load in the air and water. However, the wear volume decreases from 0.98 N to 2.94 N in HBSS and then increases with increasing dead load. The worn surface observation and chemical analysis results confirmed that corrosion wear occurred in the low load range. The magnitude of wear was [HBSS] > [air] > [water] in the low load range (0.98 N ~ 1.96 N) and [air] > [HBSS] > [water] in the high load range (2.94 N ~ 5.88 N). In terms of specific wear, the value in water and air correlates with material hardness, whereas in HBSS, it does not necessarily correlate with hardness. Obtained results are suggested that the volume loss due to corrosion has as much or more influence than wear in the low load range. From the corrosion test, it was found that the volume loss obtained from the corrosion test was smaller than that obtained from the corrosion wear. The anodic polarization curves showed that the low vertical load (0.98 N) was less corrosion-resistant than the high vertical load (2.94 N). It was suggested that $Cl^-$ ions contributed to the overall increase in wear, and $HCO_3^-$ contributed to the increase in wear in the low load range.

*Keywords: magnesium alloys, sliding wear, tribocorrosion, biomaterial.*

# Effect of microstructure on tensile properties of Mg-Al-Zn alloy in humid air

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## Abstract

Magnesium alloys have been known to be susceptible to stress corrosion cracking (SCC), which is based on hydrogen embrittlement. In the present study, AZ61 magnesium alloy was subjected to various heat treatments and the tensile properties were evaluated by a slow strain rate tensile testing at room temperature in two environments: humid air(HA) with relative humidity of 90% or above and dry nitrogen gas (DNG) atmosphere with relative humidity of 5% or less. The elongation of the specimens in HA was smaller than that in DNG. SEM observation revealed that fracture surfaces were covered with fine dimples in DNG, while quasi-cleavage fracture in HA. The degradation of ductility of the specimens with discontinuous precipitates was larger than that of the specimens with continuous precipitates.

*Keywords: Mg-Al-Zn alloy, humid air, slow strain rate technique, stress corrosion cracking, quasi-cleavage fracture*

# The influence of mischmetal (Ce, La) on the corrosion properties of AZ91 - Ca - Y alloy

**Wen Ding**[1], Jun Ho Bae[2], Hongxiu Liu[3], Sang Eun Lee[4], TaeKyung Lee[5], Bong Sun You[6*]

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**Abstract**

The influence of mischmetal (MM) addition on the microstructure and corrosion behavior of AZ91 - Ca - Y based alloy was investigated via morphology observation, phase characterization, immersion and electrochemical tests. The experimental results suggested that MM alloying can improve the corrosion resistance of AZ91 - Ca - Y. The microstructure of the as-cast alloys was found to be α-Mg, $Al_8Mn_4Y$, β-$Mg_{17}Al_{12}$ and $Al_4$(La, Ce) phases, and the morphology of $Al_4$(La, Ce) phase varies with different MM additions. The immersion and electrochemical test results showed that the corrosion resistance, pitting potential, film and charge transfer resistances of AZ91 - Ca - Y alloy increased with increasing addition of MM up to 0.3 wt.%, above which, they decreased. Surface analyses indicated that MM promoted the formation of passive films and the refinement of the precipitates and matrix grains.

*Keywords: Magnesium alloys, Corrosion, Mischmetal, Microstructure.*

# Technical **Oral Session _ Session 12**

## **Symposium D :** Light Metals and Alloys

**Light Metals and Alloys 12-2 (D12-2)** **14:00 -15:25, Nov. 23**

**Chair :** Qiaoyan Sun ( Xi'an Jiaotong University), Nokeun Park (Yeungnam University) 301, 3F

14:00-14:20 **I-D0168** **[Invited] R & D of Some New High Strength Titanium Alloys in China**
Yongqing Zhao (Northwest Institute for Nonferrous Metal Research, China)

14:20-14:40 **I-D0414** **[Invited] Synergistic relationship on the microstructure evolution and strength-toughening mechanism in a newly developed Ti-5321 Alloy**
Cong Wu (Shaanxi University of Science and Technology, China)

14:40-14:55 **O-D0627** **Effects of solute hydrogen, hydride phase formation and strain rate on hydrogen embrittlement in Ti6Al4V alloy**
Tien-Dung Nguyen (Chungnam National University, Korea)

14:55-15:10 **O-D0229** **Formation and annihilation of twinning in Ti35 alloy applied in nuclear industry during high temperature straining and annealing**
Jianping Xu (Xi'an Rare Metal Materials Institute Co. Ltd., China)

15:10-15:25 **O-D0519** **Fretting wear mechanism and anti-fretting wear by laser cladding of the titanium alloys**
Ke Hua (Northwestern Polytechnical University, China)

# R & D of Some New High Strength Titanium Alloys in China

**Yongqing Zhao**

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**Abstract**

High strength Ti-alloy is of one the important branch of Ti-alloys. Ti-alloys with strength over 1100MPa are paid great attentions. This paper reviews the R & D of some new high strength Ti-alloys in China, including high strength (≥1100MPa) high toughness TC21 alloy with damage tolerance, high strength (≥1200MPa) high toughness Ti-5321 alloy, super high strength (≥1350MPa) high toughness Ti-1300 alloy, super high strength (≥1500MPa) Ti-1500 and Ti-1600 alloys , and also the high strength Ti-12LC alloy with low cost. Among the new alloys, TC21 has become the mainstay Ti-alloy for aircrafts; Ti-1300 and Ti-12LC alloys were used for aviation, aerospace and weapons. Ti-5321, Ti-1500 and Ti-1600 alloys were just researched, and they are still in Lab. scale.

*Key words: high strength titanium alloy, mechanical property, damage tolerance titanium alloy, application*

# Synergistic relationship on the microstructure evolution and strength-toughening mechanism in a newly developed Ti-5321 Alloy

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## Abstract

Strengthen-toughening mechanism in material science is the basis for designing new alloy system and deeply exploring existing alloy systems. It is very important to reveal the phase transformation mechanism, microstructure evolution rules and their relationship with Ti-5321 service property. Research results have revealed the dissolution and precipitation rule of α phase during non-isothermal process. On this basis, three typical microstructures are tailored and the impact toughness of Ti-5321 alloy is significantly improved. Thus, the synergistic regulation of both microstructure and strength-toughness of Ti-5321 alloy is realized.

The dissolution sequence of α phase in bi-modal microstructure is as follows: secondary α phase → lamellar α phase → grain boundary α phase → equiaxed α phase. The phase transformation sequence of β-quenched microstructure during continuous heating is β+ω→β+ω+α→β+α. The microstructure formed after β heat treatment with different cooling rates show regular changes. Bi-lamellar microstructure is formed at low cooling rate, fine lamellar microstructure is formed at medium cooling rate and the metastable microstructure is formed at high cooling rate, which are related to the competitive growth mechanism among $\alpha_{GB}$, $\alpha_{WGB}$ and $\alpha_{WI}$. According to the above microstructure evolution rules, bimodal microstructure (BM), trimodal microstructure (TM) and bi-lamellar microstructure (BLM) are obtained, the corresponding impact toughness are 11.25 J·cm$^{-2}$, 25 J·cm$^{-2}$ and 37.5 J·cm$^{-2}$, respectively. The tensile strength of BLM can maintain 1050 MPa, which shows the best combination of strength and toughness.

*Keywords: Titanium alloys with high strength and toughness; Phase transformation; Microstructure evolution; Impact toughness*

# Effects of solute hydrogen, hydride phase formation and strain rate on hydrogen embrittlement in Ti6Al4V alloy

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## Abstract

Hydrogen embrittlement (HE) is a common phenomenon that deteriorates the performance of metallic materials. In this work, the HE of Ti6Al4V (Ti64) alloy was comprehensively examined by experimentally-electrochemical hydrogen charging and associated mechanical tests. Two current densities were applied as a charging method to activate solute hydrogen and hydride phase formation, from which microstructural analysis demonstrated that hydrogen accelerated the formation of crack initiation. Furthermore, nanoindentation measurements were carried out to distinguish individual micro-mechanical behaviours among a base metal, solute hydrogen and hydride phases. The results revealed different local strains that account for distinct macro-mechanical behaviours. By controlling the applied current density and strain rate, it was revealed to elucidate how hydrogen influenced the mechanical properties of the Ti64 alloy.

*Keywords: Ti6Al4V, hydrogen embrittlement, solute hydrogen, hydride phase, strain rate sensitivity*

# Formation and annihilation of twinning in Ti35 alloy applied in nuclear industry during high temperature straining and annealing

**Jianping Xu[1],** Chengze Liu[1], Jinping Wu[1], Yusheng Zhang[1], Yongqing Zhao[2*]

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**Abstract**

Due to the outstanding long-term corrosion resistance of Ti35(Ti-6Ta in wt.%) alloy in the simulated corrosion medium of the reprocessing dissolver and its excellent processing, plasticity, toughness and weldability, it has been successfully applied in industrial reprocessing equipment in China.

In this study, the evolution of microstructure and twinning of Ti35 alloy during plastic deformation at high temperature was investigated by scanning electron microscope (SEM), electron backscattered diffraction (EBSD) as well as transmission electron microscopy (TEM), aiming to reveal the formation and annihilation behavior of deformation twinning. Moreover, the influence of twinning and deformation reduction on mechanical properties of Ti35 alloy was elaborated using micro-hardness and tensile tests.

Results showed {10-12}<10-1-1>, {11-22}<11-2-3> and {10-11}<10-1-2> twins were developed during hot rolling and their proportion varied with the amount of deformation. The fraction of twinning boundary reached peak value in the 50% reduction sample, which dominated by {10-12}<10-1-1> and {11-22}<11-2-3> twins. After annealing, the deformation twins in >50% reduction samples were nearly annihilated. The twins and substructures acted as nucleation point for static recrystallization, resulting in twins annihilated and grain refinement during annealing. Micro-hardness and tensile tests revealed that deformation twinning improved strength and plasticity of the Ti35 alloy by introducing extra interfaces and reorientation.

*Keywords: Reprocessing; Ti35 alloy; Deformation twinning; Twins annihilation; Microstructure evolution*

# Fretting wear mechanism and anti-fretting wear by laser cladding of the titanium alloys

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## Abstract

Titanium alloy is widely used in aviation industry manufacturing. However, fretting wear of titanium alloy is easily happened during service environment, leading to the failure of some key parts. In addition, the fatigue limit of parts is significantly reduced after fretting, which seriously restricts the reliability and life of the alloy. Therefore, revealing the fretting behaviour of titanium alloy and improve its fretting damage resistance is one of the key problems to be solved for titanium alloy. In this project, the fretting wear properties of alloys with different α precipitated phase characteristics under different fretting working conditions were studied, and the internal correlation between the precipitated phase characteristics and the initiation and propagation of wear cracks was established to reveal the fretting wear mechanism of titanium alloy. On this basis, based on the laser cladding technology, 2-3 kinds of anti-fretting coatings were designed, and the fretting wear behaviour and mechanism of the coatings were demonstrated. This work can provide theoretical and scientific basis for improving the fretting wear resistance of titanium alloys.

*Keywords: Titanium alloy, fretting wear, laser cladding.*

# Technical **Oral Session _ Session 12**

## **Symposium K :** High-Entropy Materials and Amorphous Materials

**High-Entropy Materials and Amorphous Materials 12 (K12)** **14:00 -15:30, Nov. 23**

**Chair :** Chuang Dong (Dalian Jiaotong University) Samda Hall B, 3F

14:00-14:15 **O-K0599** **Tailoring microstructure and corrosion behavior of CoNiVAlx medium entropy alloys via Al addition**
Zhimin Pan (University of Science and Technology Beijing, China)

14:15-14:30 **O-K0140** **Wear-resistant CoCrNi multi-principal element alloy at cryogenic temperature**
Qing Zhou (Northwestern Polytechnical University, China)

14:30-14:45 **O-K0210** **Mechanical Properties, Oxidation Resistance, and Tribological Performance of AlCrNbTaTi Refractory High-Entropy Alloys**
Xiaolin Li (Northwestern Polytechnical University, China)

14:45-15:00 **O-K0134** **Enhancing magnetic properties of the Co66Fe6Si13B15 metallic glass through DC current annealing**
Caiyun Liu (University of Science and Techology Beijing, China)

15:00-15:15 **O-K0350** **A new strong pearlitic multi-principal element alloy to withstand wear at elevated temperatures**
Wenwen Sun (Southeast University, China)

15:15-15:30 **O-K0682** **Strong yet strain-hardenable equiatomic CoCrFeMnNi high-entropy alloys by dynamic heterostructuring**
Jungwan Lee (Pohang University of Science and Technology, Korea)

# Tailoring microstructure and corrosion behavior of $CoNiVAl_x$ medium entropy alloys via Al addition

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## Abstract

The effect of Al addition on the microstructure and corrosion behavior of $CoNiVAl_x$ medium entropy alloys (MEAs) was investigated. Results indicated that increasing Al addition leaded to the increase in the atomic ratio of Al/V and $O^{2-}/OH^-$, which implied that Al addition promoted the increase of metallic oxide in the film, thus enhancing the stability and protection of the passive film. The enhanced corrosion resistance caused by Al addition might be attributed to the dominant role of Al in stabilizing the passive film. The difference in the Volta potentials of FCC and BCC phases indicated the existence of microgalvanic coupling, which suggested that the BCC phase served as a localized cathode while the FCC matrix and FCC lath acted as anodes. This accounted for the pitting mechanism of $CoNiVAl_x$ MEAs via Al addition. The current work can provide some guidance in assessing the corrosion resistance of alloy systems containing precipitates.

*Keywords: Medium entropy alloy; Corrosion resistance; Microstructure; Precipitate; Passive film.*

# Wear-resistant CoCrNi multi-principal element alloy at cryogenic temperature

Qing Zhou (Northwestern Polytechnical University)

**ABSTRACT**

Traditional high strength engineering alloys suffer from serious surface brittleness and inferior wear performance when servicing under sliding contact at cryogenic temperature. Here, we report that the recently emerging CoCrNi multi-principal element alloy defies this trend and presents dramatically enhanced wear resistance when temperature decreases from 273 K to 153 K, surpassing those of cryogenic austenitic steels. The temperature-dependent structure characteristics and deformation mechanisms influencing the cryogenic wear resistance of CoCrNi are clarified through microscopic observation and atomistic simulation. It is found that sliding-induced subsurface structures show distinct scenarios at different deformation temperatures. At cryogenic condition, significant grain refinement and a deeper plastic zone give rise to an extended microstructural gradient below the surface, which can accommodate massive sliding deformation, in direct contrast to the strain localization and delamination at 273 K. In addition, the temperature-dependent cryogenic deformation mechanisms (stacking fault networks, twinning and phase transformation) are also revealed, which provide additional hardening and toughening of the subsurface material. The current work clarifies the superior wear resistance of the CoCrNi alloy, making it an excellent candidate for safety-critical applications involving cryogenic sliding conditions.



BIO: Dr. Qing Zhou received his Ph.D. degree in material science and engineering from Xi'an Jiaotong University, China, in 2017. After that, he has worked at Northwestern Polytechnical University, China, as an associate professor. His research areas cover design, fabrication, and characterization of high-performance alloy materials, modeling and simulation of tribological behavior of metal composites, etc. He can be reached by email: zhouqing@nwpu.edu.cn.

# Mechanical Properties, Oxidation Resistance, and Tribological Performance of AlCrNbTaTi Refractory High-Entropy Alloys

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## Abstract

The mechanical, oxidation resistance, tribological behavior of a series of AlCrNbTaTi refractory high-entropy alloys was systematically investigated from room temperature to elevated temperature. The relationship between the alloy composition, microstructure, mechanical properties, oxidation resistance and tribological performance was analyzed. The results shows that all the three alloys have a bcc single-phase structure. The Ta addition enhances solid solution strengthening and increases the melting point that would resist high-temperature thermal softening. As a result, high-temperature strength is enhanced considerably, the coefficients of friction (COF) and wear rates of the alloys are reduced considerably at elevated temperatures, demonstrating excellent friction-reducing and anti-wear properties, e.g., the COF and wear rate of $AlCr_{0.5}NbTaTi_3$ alloy at 800 ℃ are 0.34 and $4.40\times10^{-7}$ $mm^3/N\cdot m$, respectively. The excellent wear resistance at high temperatures can be attributed to the existence of an oxide-tribo layer ($Ta_2O_5$ and $TiO_2$) with ultrafine-grained layers and the good high temperature mechanical properties.

*Keywords: Refractory high entropy alloys; High temperature; Mechanical properties; Oxidation resistance; Wear resistance; Oxide-tribo layer*

# Enhancing magnetic properties of the $Co_{66}Fe_6Si_{13}B_{15}$ metallic glass through DC current annealing

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## Abstract

Co-based metallic glasses have good soft magnetic properties, then possess numerous potential utilizations. However, the large cooling rate that needs for amorphous state leads to large internal stress and structural heterogeneity, proper heating treatment is required. to eliminate the internal stress and improve magnetic performance,

In this study, the $Co_{66}Fe_6Si_{13}B_{15}$ MG was annealed by direct current (DC) with current density ranging from 67 A/mm$^2$ to 333 A/mm$^2$ for different times. When the current density is smaller than 167 A/mm$^2$, the magnetization ($M_s$) increases from 43 emu/g to over 60 emu/g, accompanied by sharp decline of coercivity ($H_c$). The best soft magnetic performance with $M_s$ of 72 emu/g and $H_c$ of 4 Oe was obtained in the sample after annealed with current density of 217 A/mm$^2$ for 60 s. Larger grains result in the deterioration of magnetic properties when the current density exceeds 233 A/mm$^2$.

Similarly, the effect of both single- and two-step DC annealing procedures on the giant magneto-impedance (GMI) of glass-coated $Co_{66}Fe_6Si_{13}B_{15}$ amorphous wires were further studied. The magnetic properties initially increased with increasing current intensity and reached a peak value before declining at larger current intensity for both methods. An maximum improvement of the GMI ratio by about 5 times was obtained for a two-step DC annealed sample, while that was only 2.44 times for single-step annealed samples. This could be attributed to the more homogeneously distributed precipitations in the matrix caused by the two-step procedure.

The obtained results indicate that high-density but short-time current annealing is a very efficient method to improve magnetic properties, which satisfies the demand of industrial application.

*Keywords: metallic glass; magnetic property; direct current annealing;* giant magneto-impedance.

# A new strong pearlitic multi-principal element alloy to withstand wear at elevated temperatures

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## Abstract

Alloys with high wear resistance at elevated temperatures are highly desired for modern application under extreme working conditions. Conventionally, nano-layered pearlitic structure could greatly improve the strength and wear resistance for steels, but they are not heat resistant. Therefore, it is promising to make a new pearlite structure that could withstand heat. In this study, we revitalize the pearlite structure by inheriting it from single principal element iron alloys into a newly developed multi-principal element alloy (MPEA) through a classic eutectoid reaction, producing a nanometre sized layered microstructure. Taking advantages of the thermal stability of MPEAs, formation of strong pearlite not only significantly improves the room temperature wear resistance of the MPEA, more importantly, it endues the MPEA with excellent elevated temperature strength and wear resistance. Therefore, pearlitic structure is a direction worthy of pursuing in microstructural design of high performance MPEAs.

*Keywords: Multi-principal element alloy (MPEA); Layered structure; Pearlite; Wear resistance.*

# Strong yet strain-hardenable equiatomic CoCrFeMnNi high-entropy alloys by dynamic heterostructuring

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## Abstract

Heterostructuring gives solutions to achieve better mechanical performance of metallic materials. For instance, partial static recrystallization by short-term annealing induces bimodal grain size distribution. Distinct from the well-studied 'static heterostructuring' by cold rolling followed by annealing, this study introduces 'dynamic heterostructuring' by hot rolling. Dynamic recrystallization (DRX) during the hot rolling as a softening mechanism leaves room for dislocation accumulation. With the expectations of enhanced strain hardening of the as-rolled materials with the aid of the DRX, we monitored tensile responses of the as-hot-rolled equiatomic CoCrFeMnNi high-entropy alloys (HEAs). Among the hot rolling temperatures from 800 ℃ to 900 ℃ with a thickness reduction ratio of 78.6% for the HEAs, the hot rolling at 850 °C results in a bimodal grain size distribution, i.e., partial DRX. It comprises relatively fine DRXed grains and coarse unrecrystallized grains: the latter is harder than the DRXed ones with relatively low dislocation density. The microstructural heterogeneity results in uniform elongation of ~13% due to the accumulation of dislocations at the grain boundaries inside the soft DRXed grains. This endows the as-hot-rolled single-phase HEAs with strain hardenability without the aid of phase transformation, deformation twinning, or precipitates. In addition, the hot-rolled HEAs with high dislocation density have doubled yield stresses of those of conventionally cold-rolled and annealed counterparts. Considering the industrial benefits of the simplified thermo-mechanical control processes, this work extends the academic and practical value of DRX by dynamic heterostructuring through annealing-free hot-rolling.

*Keywords: Dynamic recrystallization, high-entropy materials, grain boundary, mechanical properties, dislocation*

# **Symposium P** : Satellite Symposium

4th KIM-CSM symposium: New Metal Materials: Low-carbon emission, New energy vehicles & Lightweights

November 23, 9:00-15:30

401, ICC jeju

# **Symposium P** : Satellite Symposium

## **Symposium P :** 4th KIM-CSM symposium: New Metal Materials: Low-carbon emission, New energy vehicles & Lightweights

### New Metal Forming Process & Properties (P1) — 09:00 -10:40, Nov. 23

**Chair :** Opening - Hyoungwook Kim (Korea Institute of Materials Science) — 401, 4F
ShiHoon Choi (Sunchon National University)

09:00-09:10 **Opening Ceremony** **Welcome Message**
KIM President, CSM president (Video)

09:10-09:40 **I-P0819** **[Keynote] Electric Current Assisted Processing and its Mechanism**
Heung Nam Han (Seoul National University, KIM)

09:40-10:00 **I-P0829** **[Invited] Crash Cracking Index and Hydrogen Embrittlement Mechanisms of Hot Stamping Components**
Hongzhou Lu (CITIC Metal Co., LTD, CSM)

10:00-10:20 **I-P0000** **[Invited] Elasto-visco-plastic self-consistent polycrystal model for finite element simulations of bending and springback**
Youngung Jeong (Changwon National University, KIM)

10:20-10:40 **I-P1013** **[Invited] Al-Si Coated Press Hardened Steel with Improved Bendability**
Hongliang Yi (Northeastern University, CSM)

# Electric Current Assisted Processing and its Mechanism

Heung Nam Han

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**Abstract**

Electroplastic phenomenon has been demonstrated by that the elongation increases remarkably during deformation under electric current without significant temperature rise due to Joule heating. Since the 1960s, electroplasticity has been actively investigated; however, full explanation of electroplasticity mechanism has been lacking. In this presentation, the origin of electroplasticity is elucidated based on numerical and experimental approaches. Ab-initio calculations show that a charge imbalance near defects weakens drastically atomic bonding. The electroplastic behavior could be well reproduced with microstructure-based FE simulations. In addition, the weakening of atomic bonding was confirmed by measuring elastic modulus under electric current, which is inherently related to bond strength. As a fundamental approach of electroplasticity, we investigated the effect of electric current density on recrystallization kinetics of ultra-low carbon steel through the microstructure characterization and mechanical property analysis. A single pulse treatment (SPT) with different electric current densities and appropriate durations was utilized to achieve a target peak annealing temperature. The dependence of the athermal effect in the SPT recrystallization on the current density was quantified by introducing effective activation energy and effective temperature. We believe that the novel approach presented in this study can be extended to other electric current-induced phenomena in metallic materials. As one of the applications of electroplasticity, we utilized sub-second electric pulsing, which can enhance the kinetics of microstructural change to infinitely reset the damaged microstructure as a non-autonomous self-healing method. Besides, various application examples such as electric current assisted trimming, joining, sintering, etc. will be introduced in this presentation.

*Keywords: Electroplasticity; Athermal effect; Self-healing; Electric Current; Dislocation density;*

# Crash Cracking Index and Hydrogen Embrittlement Mechanisms of Hot Stamping Components

**Hongzhou Lu**[1], Aimin Guo[1], Yi Feng[2], Yan Zhao[3], Wenjun Wang[1], Gang Fang[2], Yisheng Chen[4], Wei Li[5]

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## Abstract

Press-hardening steel (PHS) and hot stamped parts have insufficient toughness and potential hydrogen embrittlement issues, especially for coated and 1800-2000MPa PHS and hot stamping parts. Firstly, the use of Nb, Nb-V and Nb-Mo microalloying have refined the grain size of PHS and decrease the banded structure, increased the bending angle of the steel and the critical fracture strain of the parts under the stress triaxiality of 0.4-0.6, thereby improving the collision fracture index of the parts. This has been verified through comparative experiments on the drop weight of the parts, and realized a closed-loop system of material cold bending angle, fracture material card, part collision experiment, and part fracture index. Secondly, through microalloying and process control, small-scale nano-size NbC high-energy hydrogen traps are achieved, the unit grain boundary hydrogen distribution is reduced after grain refinement, and the austenitizing time is reduced to reduce reduction hydrogen generation reactions. The significant improvement in hydrogen embrittlement resistance of parts is achieved, which has been verified through U-shaped constant load bending experiments. At the same time, the new material and process can achieve the same hydrogen embrittlement resistance as traditional materials without dew point control. The above-mentioned Nb-bearing PHS are widely used in passenger car body components, commercial vehicle compartments, and commercial vehicle hot formed wheels, improving the automotive safety performance.

*Keywords: Safety; Hydrogen embrittlement; Lightweight; Hot Stamping; Niobium*

# Al-Si Coated Press Hardened Steel with Improved Bendability

**Hongliang Yi[1,2],** Dapeng Yang[1], Shu Zhou[2], Linlin Zeng[1]

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## Abstract

Press hardened steels (PHS) are increasingly used for vehicle body structure components due to their high strength and excellent formability. To prevent oxidation and decarburization of the steel surface during the high-temperature hot stamping process, an Al-Si coating is commonly employed on the PHS surface. The initial coating thickness is typically 25 μm, after hot stamping, the Al-Si coating transforms into several intermetallics layers and a ferrite (α) diffusion layer between intermetallics and the martensite (α′) substrate. Al-Si coated PHS always has lower bending angle than its bare counterpart, which limited the application of PHS on autobody. The physical essence of the effect of Al-Si coating on the bendability of PHS is unclear and there still lack of effective ways to improve the bendability of PHS. In the present work, we found that the α′ substrate surface which close to the α layer was rich in C due to the interface migration of the Al-Si coating and the PHS substrate, and then microcracks are easy to form from the brittle high C martensite during bending deformation, leading to bendability deterioration of the Al-Si coated PHS compared to the bare steel plate. Based on the above findings, a method by tailoring coating thickness to reduce the C enrichment of the α/α′ interface was proposed to improve the bendability of Al-Si coated steel. The bending angle increases from 54.2° to 65.4° by reducing the coating thickness from 25 μm to 10 μm. Interestingly, the paintability and corrosion resistance of the thinner coating kept the same as the thick ones. In addition, a thinner Al-Si coating can also lower material cost, shorten austenitizing heating time and reduce electrode wear during resistance spot welding. This work will change the industry practice of PHS and have a significant impact on the global automobile industry.

*Keywords:* Lightweight of automobile; Press hardened steel; Al-Si coating; Bendability; Interfacial carbon enrichment

# **Symposium P** : Satellite Symposium

## **Symposium P :** 4th KIM-CSM symposium: New Metal Materials: Low-carbon emission, New energy vehicles & Lightweights

### Green Metal Forming & Properties (P2) — 10:50 -12:10, Nov. 23

**Chair :** Hongzhou Lu (CITIC Metal Co., LTD) — 401, 4F

10:50-11:10 **I-P0000** **[Invited] Simulating cyclic loading behaviour of a magnesium alloy at elevated temperature**
Hyuk Jong Bong (Korea Institute of Materials Science, KIM)

11:10-11:30 **I-P0909** **[Invited] The hydrogen embrittlement behaviours of micro-alloyed press hardened steel: mechanical property, microstructure characterization and modelling**
Yan Zhao (Beijing Institute of Technology Chongqing Innovation Center, CSM)

11:30-11:50 **I-P0996** **[Invited] Deciphering the effect of initial texture on the hemming performance of AA5083 aluminum alloy**
ShiHoon Choi (Sunchon National University, KIM)

11:50-12:10 **I-P0872** **[Invited] Latest Progress of Light weight and Low CO2 Emission Solutions for New Electric Vehicle**
Fei Han (Automotive Steel Institute, CSM)

# The hydrogen embrittlement behaviours of micro-alloyed press hardened steel: mechanical property, microstructure characterization and modelling

**Yan Zhao[1]**, Lintao Gui[2], Jian Wang[3], Hongzhou Lu[4]

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## Abstract

Press hardened steel (PHS) significantly contributes to the light weight of automotive, which reduces the energy consumption as well as the carbon emission. However, the lath martensite in PHS is sensitive to hydrogen embrittlement (HE). In this study, a novel Nb-V bearing PHS was developed (22MnB5NbV) to address HE problem. The HE property was tested in an experiment that integrated the VDA 238-100 tight radius bend test and the acid solution. The duration time of 22MnB5NbV in the test was apparently improved in comparison with 22MnB5. The TEM result indicated the size of the lath martensite is reduced from 0.35 μm to 0.15 μm after the addition of Nb and V. Large amounts of nano-scale particles in the lath martensite were identified as the Nb-V precipitates via TEM-EDS. The 3D atom probe tomography showed the precipitate had a core-shell structure, in which Nb played the role of nucleation site, and accounted for a much larger proportion compared to V. The similar result for the element precipitation proportion was also found in the leaching experiment. Molecular dynamics method can determine the energetics and mobility of a single defect (dislocation, vacancy, crack, etc.) or atom, which has been applied in HE simulation. In this study, the dynamic interaction between H atom and dislocation was introduced. Meanwhile, the Fe-C-Nb-H MEAM function was developed and used in H absorption by the NbC precipitate or the NbC/matrix interface.

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*Keywords: Press hardened steel, hydrogen embrittlement, micro-alloyed method, Molecular dynamics, precipitation*

# Deciphering the effect of initial texture on the hemming performance of AA5083 aluminum alloy

**Preetham Alluri, Aman Gupta, Abhishek Kumar Singh, Shi-Hoon Choi***

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## Abstract

The hemming process is widely utilized in the automotive industry to shape aluminum sheets through 180-degree bending operations, ensuring the absence of cracks or surface defects. However, the current state of AA5083 aluminum alloys, which exhibit a higher strength-to-weight ratio, often renders them susceptible to failure during hemming. While the initial crystallographic texture of aluminum significantly influences its deformation behavior and prevents surface defects, the complete correlation between crystallographic texture and hemming performance has yet to be fully explored. This study aims to comprehend the impact of various texture components on the hemming behavior of commercial AA5083 aluminum alloy sheets under ambient temperature conditions. The data obtained from surface roughness measurements was combined with orientation Electron Back Scatter Diffraction (EBSD) data to identify the active slip systems in the deformed microstructure. Furthermore, the study investigates the effect of Friction Stir Processing (FSP) on hemming performance. Crystal Plasticity Finite Element Method (CPFEM) simulations were conducted to discern the relationship between the texture anisotropy of neighboring grains and the development of valleys in the tension zone of the outer bent region. These CPFEM results were subsequently employed to discuss shear band formation, crack initiation, and propagation along the outer tensile zone during the hemming process.

***Keyword:*** *Aluminum alloys, AA5083, CPFEM, Crystallographic Texture, Surface roughness.*

# Latest Progress of Light Weight and Low CO2 Emission Solutions for New Electric Vehicle

**Fei Han**[1], Aihui Luo[2], Ping Bao[3]

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## Abstract

For the stricter safety and carbon neutrality requirement, Baosteel launched the latest NEV concept BIW, BCB EV Pro. Furthermore, the latest progress of Low-carbon-emission steels will be presented including the automotive sheet net zero carbon path. And the light-weight solution with one-piece integrated parts will be demonstrated also.

*Keywords: carbon neutrality, light-weight solution, UHSS, integrated door-ring*

# **Symposium P** : Satellite Symposium

## **Symposium P :** 4th KIM-CSM symposium: New Metal Materials: Low-carbon emission, New energy vehicles & Lightweights

**New Metals for Light weightening (P3)** — **13:40 -15:20, Nov. 23**

**Chair :** Hyoungwook Kim (Korea Institute of Materials Science) — 401, 4F

13:40-14:00 **I-P0896** **[Invited] The New Challenge and Replying Strategy of Early Vendor Involvement Solutions of Automotive Materials with the Goal of Carbon Neutrality**
Jia Zhou (China Automotive Engineering Research Institute Co., Ltd, CSM)

14:00-14:20 **I-P0833** **[Invited] Improvement of corrosion resistance of SEN Mg alloys**
Bong Sun You (Korea Institute of Materials Science, KIM)

14:20-14:40 **I-P0885** **[Invited] Exploration and research on key technologies of green low-carbon manufacturing for automobile aluminum alloy components under the vision of low-carbon emission**
Yu Wang (CITIC Dicastal Co.,Ltd, CSM)

14:40-15:00 **I-P0989** **[Invited] Eco-friendly high strength Al-Zn-Mg-Cu alloy sheets for automobile body application**
Hyoungwook Kim (Korea Institute of Materials Science, KIM)

15:00-15:20 **I-P0947** **[Invited] Precipitation behaviour of Al-7Si-0.35Mg casting alloy during T5 heat treatment**
Young-Hee Cho (Korea Institute of Materials Science, KIM)

# The New Challenge and Replying Strategy of Early Vendor Involvement Solutons of Automotive Materials with the Goal of Carbon Neutrality

**Jia Zhou[1],** Gang Fang[2], Guanrun Zhu[3], Junping Zhang[4]

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**Abstract**

To deal with climate change, more than more than 130 countries have proposed emission reduction targets of "net-zero emission". Automobile and their raw materials are high-emission industrial products, and OEMs and raw material suppliers are facing great pressure to reduce emissions. Meanwhile, with the industry's demand for weight reduction and cost reduction, the lightweight of automobiles have been put forward of higher levels of requirements. Therefore, the early vendor involvement solutons (EVI solutions) of should combine with cost, performance and carbon footprint in the view of whole life cycle to meet the different product orientation of OEMs. In other words, some solutions with cost first, or carbon reduction first, or lightweight first are urgent to be proposed with the tool of assessment or/and life cycle cost.

***Keywords**: Early Vendor Involvement, Carbon Neutrality, Replying Strategy, Life Cycle Assessment.*

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

# Improvement of corrosion resistance of SEN Mg alloys

**Bong Sun You**[1], Hongxiu Liu[2], Wen Ding[3], Jun Ho Bae[4]

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## Abstract

Our team have been studied on the development of new corrosion resistant magnesium alloy by the addition Ca and Y together which was named as SEN alloy. Because the alloy has excellent corrosion resistance, lots of studies have been done for commercialization, but further improvement of corrosion resistance or mechanical properties is required for much wider application. In this paper, in order to further improve the corrosion resistance of SEN alloy, we tried to control the trace elements added to the alloy and change processing parameters for the microstructural optimization. Also, it introduces the mechanism of high corrosion resistance of Ca and Y containing alloys, and compares the corrosion behaviour with that of commercial alloys.

*Keywords: Mg alloy, Corrosion behaviour, Cooling rate*

# Exploration and research on key technologies of green low-carbon manufacturing for automobile aluminum alloy components under the vision of low-carbon emission

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## Abstract

Carbon neutralization is a crucial issue recognized globally for the sustainable development of human society. As the requirements on lightweight vehicles are further improved, aluminum alloy components are widely used in automobile because of the better mechanical properties, easier machinability and corrosion resistance. However, aluminum alloy components generate a large amount of carbon emissions at the raw material and manufacturing stages result from the energy structure and electrolytic process. In addition, Scrappage and recycling of aluminium alloy components resulted in a large amount of metal waste because the metal recycling mechanism and technology development is necessary to be improved. Our research team developed a key technology system from three dimensions of recycled aluminum application, green manufacturing technology innovation and energy reuse to explore the application path of green low-carbon technology in the industrialization of aluminum alloy components. The technology innovation of whole process is achieved, which meets the carbon emission production requirements of international mainstream customers and contributes to establish an industrial model.

*Keywords: Aluminum alloy components, Green low-carbon technology, Recycled aluminium, Green manufacturing, Energy reuse*

# Eco-friendly high strength Al-Zn-Mg-Cu alloy sheets for automobile body application

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## Abstract

The weight reduction of automobile body structure is an important issue for car manufactures to improve fuel economy and CO2 emission. Many high strength aluminum has been developed for automobile applications, but the cost is high for commercial usage. Twin roll casting is well known as a cost effective and low CO2 emission process to make aluminum alloy strips, however, it has been used for manufacturing several aluminum alloys with low solute contents. In order to fabricate high strength aluminum sheets, new twin roll caster designed and the process condition optimized. The cast strips has a fine grain structure and high formability during rolling process. Al-5.2wt%Zn-2.3wt%Mg-1.5wt%Cu alloy and Al-7.9wt%Zn-2.7wt%Mg-2.1wt%Cu alloy strips can be successfully fabricated by the conventional rolling and heat treatment process. The effects of the process parameters on quality of alloy strips and mechanical properties of the sheets after annealing will be discussed. In addition, for improving bake hardening response of the Al-Zn-Mg-Cu alloy sheet alloy, pre-aging treatment condition after solution heat treatment were investigated.

*Keywords: Al-Zn-Mg-Cu, Sheet, Automobile, Twin roll casting, Strength*

# Precipitation behaviour of Al-7Si-0.35Mg casting alloy during T5 heat treatment

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## Abstract

Al-Si-Mg casting alloys have been being used as heat treatable alloys and are often T6 heat treated, involving both solid-solution treatment and aging to maximize the mechanical properties. However, focus is currently shifting to T5 heat treatment, which is a direct aging after casting, due to the high operating costs as well as the distortion issues associated with solution heat treatment. T5 is a certainly cost-effective and alternative heat treatment fo industrial applications when particularly handling large single-piece castings with complexity in shapes, Tesla's Giga Casting products for instance. However, the successful implementatio of T5 heat treatment requires an in-depth understanding of the associated casting parameter and their influence on the mechanical properties and conductivities. Cooling conditions upo casting is one of the most important factors influencing the aging behaviour and the resultin mechanical properties of T5 heat-treated Al-Si-Mg alloys. While cooling rates during solidification determine the initial solubility of solute elements in the matrix, we recently found that cooling conditions even after the solidification can affect the amount of pre-precipitate (e.g., Si clusters and B′) and the subsequent aging hardening response directly after casting. Analysis of precipitation kinetics and number densities of precipitates indicates that the pre precipitation can interfere with the precipitation of β″, otherwise promoting the precipitation o coarse β′, U2 and Si, which reduced the overall T5 precipitation hardenability. Both mechanica properties and thermal conductivity of the Al-Si-Mg alloys, which are both influenced by th secondary phases and precipitates, was also investigated for the alloys with various T5 heat treatment conditions. Based on the characterization of precipitates at different aging steps wit TEM works, the interrelationships between the microstructural evolution particularly withi the matrix and the properties are further discussed.

*Keywords: Al-Si-Mg alloy; casting; T5 heat treatment; precipitation; mechanical properties thermal conductivity*

# **POSTER** Session **1**

November 20, 18:00-19:30

3F Lobby, ICC jeju

# POSTER Session 1

## Symposium A : Advanced Steels and Properties

**P-A0011** **Research and development of S22053+12MnNiVR stainless steel rolling clad plate by Ansteel**
Xin Ouyang (Anshan Iron and Steel Group Steel Research Institute, China)

**P-A0012** **Microstructure and precipitated phase changes of a Cu-Nanophase Precipitation Strengthening Steel under welding thermal cycle**
Guo Peng (AnShan Iron and Steel Group Corporation, China)

**P-A0014** **Effect of alloying elements Al and Si on high temperature oxidation behavior of 1000MPa ultra-high strength steel**
Liangliang Zhang (Shougang Group Co., Ltd, China)

**P-A0048** **Corrosion Behavior of Q500qENH Weathering Bridge Steel in a Simulated Rural Atmosphere**
PENG GAO (State Key Laboratory of Metal Material for Marine Equipment and Application, China)

**P-A0051** **Study on Corrosion Behavior of Q690qENH and 09CuPCRNi in Marine Industrial Atmospheric Environment**
Lin Li (State Key Laboratory of Metal Material For Marine Equipment And Application, China)

**P-A0054** **Corrosion Behavior of Typical Ship Plate Steels in Simulated Marine Atmospheric Environment**
Xiandong Su (Ansteel Group Corporation, China)

**P-A0069** **Microstructure control and stenghtening-toughening mechanism of 68.4GPa·% grade cold rolled steel**
Zherui Zhang (Ansteel Iron & Steel Research Intitute, China)

**P-A0497** **Effects of Stress Triaxiality Distribution on Tensile Fracture of Notched TWIP Steel Plate**
Ki-Chae Jung (Hanbat National University, Korea)

**P-A0732** **Integrated decarburization and oxidation model for high carbon-chromium containing steel**
Niladri Naskar (Seoul National University, Korea)

# **POSTER** Session **1**

**P-A0971** **Hydrogen embrittlement of 300-series stainless steels under cryogenic conditions**
Yoonmoon Chung (Hanyang University, Korea)

**P-A0973** **Designing lightweight Co-free maraging steels**
Chae Young Kim (Hanyang University, Korea)

**P-A0980** **The relationship between thickness depth and hydrogen embrittlement in pipeline steel**
Hyun Wook Lee (Hanyang University, Korea)

**P-A1003** **Comparison of Microstructural and Mechanical properties of Weld Joints in 9% Ni steel Prepared with Ni-based and Fe-based Filler Materials**
Kwangsu Choi (Korea Institute of Industrial Technology, Korea)

| P-A0011 |

# Research and development of S22053+12MnNiVR stainless steel rolling clad plate by Ansteel

**Ouyang Xin**[1], Hu Xinming[2], Sun Diandong[3], Wang Chu[4], Xing Mengnan[5], Liu Chenxi[6]

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## Abstract

This paper describes the development process of S22053+12MnNiVR composite steel plate using vacuum electron beam welding technology and double-sided symmetrical billet assembly method in ANSTEEL Co., Ltd., which has a product thickness of 2+12mm and is used in multi-stage flash seawater desalination evaporator shell. The stainless-steel clad steel plate has excellent comprehensive mechanical properties, good resistance to intergranular corrosion and seawater corrosion. The bonding rate of its composite interface meets the requirements of GB/T 8165-2008 Class I, and the bonding rate between atoms is 100%. As a new generation of green composite material, the successful development of S22053+12MnNiVR stainless steel-clad steel plate is of great significance in reducing the cost of seawater desalination, increasing the life of seawater desalination equipment, and realizing the localization of equipment, which provides an important way for China to solve the shortage of fresh water resources and lays a solid foundation for China to realize the green recycling of seawater resources.

**Keywords:** Seawater desalination;Vacuum electron beam welding technology;Rolling compound;Stainless steel clad steel plate

| P-A0012 |

# Microstructure and precipitated phase changes of a Cu-Nanophase Precipitation Strengthening Steel under welding thermal cycle

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## Abstract

The welding heat affected zone of copper precipitation strengthening steel is an important part of the welded joint, and it's microstructure plays an important impact on the joint properties. In this paper, the effect of welding heating and cooling process on the microstructure and precipitates of copper precipitation strengthened steel is simulated by welding thermal simulation test. Vickers hardness tester is used to measure the hardness distribution of the sample, impact test is used to measure the low-temperature toughness under different parameters, and the changes of the matrix structure and precipitated phase of the thermal simulation sample are observed by metallography, transmission electron microscopy and other methods. After the welding thermal cycle, the hardness of the matrix changes with the increase of T8/5 and the decrease of the peak temperature. The matrix structure changes from upper bainite and granular bainite to granular bainite and ferrite. The copper precipitate on the matrix undergoes the process of re-dissolving and precipitation under the action of welding thermal cycle. The rapid heating and cooling process reduces the size of the nano-phase re-precipitated at the dissolution position of the original precipitate.

**Key words:** Copper precipitation strengthening steel; Welding thermal cycle; Welding thermal simulation; Copper nanometer precipitation phase

| P-A0014 |

# Effect of alloying elements Al and Si on high temperature oxidation behavior of 1000MPa ultra-high strength steel

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## Abstract

The oxidation behavior of 1000MPa ultra-high strength steel at high temperature was studied by thermogravimetric analysis; The influence of alloying elements Al and Si on the morphology and structure of oxide scale was discussed, and the distribution of alloying elements at the interface between oxide scale and matrix was analyzed. The influence of C element in steel on intergranular oxidation was also described. The results show that when the temperature is 1000-1100°C,because of the addition of 0.4% (mass fraction, the same below) Al and 0.4% Si in the steel , there is a discontinuous Al-Si enriched particle zone at the interface between the oxide scale and the matrix; When the temperature exceeds 1100°C, the Al-Si enriched particle belt becomes c ontinuous and liquefaction occurs at the same time. In the subsequent cooling process, on the one hand, Al and Si elements continue to diffuse into the oxide scale,which inhibiting the transformation of FeO, making the FeO content in the oxide scale structure as high as 20-30%; on the other hand, Al and Si elements diffuse into the matrix, eroding the grain boundary and causing the occurrence of intergranular oxidation. In particular, because the steel contains 0.2% C, the presence of Si and Al increases the decarburization tendency of the steel, increases the grain size, and the grain boundary channel is longer, which provides a powerful channel for the diffusion of Si and Al elements along the grain boundary, making the intergranular oxidation depth reach 10-15μm.

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**Keywords:** ultra-high strength steel; enriched particle; decarburization; intergranular oxidation

Poster Session 1

# Corrosion Behavior of Q500qENH Weathering Bridge Steel in a Simulated Rural Atmosphere

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## Abstract

The corrosion behavior of Q500qENH weathering bridge steel in a laboratory simulated rural atmosphere was investigated by means of cyclically alternative immersion-drying accelerated corrosion test, the morphology and composition characterization of rust, and the electrochemical impedance spectroscopy analysis. The results show that the steel presented characteristics of uniform corrosion. The corrosion kinetics of Q500qENH weathering bridge steel accorded with a power function, and the corrosion process of the Q500qENH weathering bridge steel can be divided into two stages: acceleration and deceleration. The corrosion products were transformed from α-FeOOH and Fe3O4 to α-FeOOH and γ-FeOOH with the progress of corrosion process, while the charge transfer resistance and the rust layer resistance were increased. Besides, Cu, Cr and Ni were involved in the formation and evolution of rust layers.

**Keywords:** weathering bridge steel; rural atmosphere; corrosion behaviour; corrosion products

| P-A0051 |

# Study on Corrosion Behavior of Q690qENH and 09CuPCRNi in Marine Industrial Atmospheric Environment

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## Abstract

The corrosion behavior of Q690qENH weathering bridge steel and 09CuPCrNi weathering steel in the marine industrial atmospheric environment of the Bayuquan factory area of Ansteel was studied by means of corrosion loss method, electrochemical analysis method, macroscopic morphology observation method, SEM and XRD. The results showed that the average annual corrosion depth of Q690qENH in 4 years was 0.033 mm/a, and the average corrosion rate of 09CuPCRNi was 0.054 mm/a. Compared with 09CuPCRNi, Q690qENH had obvious internal and external rust layer structure, and the corrosion pit depth

was shallow after rust removal. Q690qENH exhibited good corrosion resistance, which was attributed to the low electrochemical activity of the substrate surface and the rust layer structure with strong protection. The corrosion phase composition of Q690qENH and 09CuPCrNi were α-FeooH, β-FeooH, γ-FeooH, and Fe3O4. Q690qENH rust layer protection coefficient α/γ* value was higher, indicating that the protection of the rust layer was better.

**Key words:** weathering bridge steel; atmospheric corrosion; rust layer;corrosion behavior

| P-A0054 |

# Corrosion Behavior of Typical Ship Plate Steels in Simulated Marine Atmospheric Environment

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## Abstract

The corrosion behavior of ship plate steels A, AH32 and AH36 in marine atmospheric environment simulated by cyclic immersion experiments was studied. The results of corrosion kinetics analysis indicate that with the increase of NaCl concentration in the cyclic immersion test solution, the corrosion ability of solution for steels increases first and then decreases, and the corrosion of steels is the most serious in 3.5% NaCl solution. The corrosion morphology and composition analysis shows that with time going on, the rust layer on the sample surface thickened gradually and lots of rust cells formed. A number of cracks and pores existed in the rust layer, and many corrosion pits could be seen after the removal of rust cells.The rust layer was enriched with Mn, and the transformation from β-FeOOH to γ-FeOOH and α-FeOOH occurs, which increases the stability of the rust layer. Through the electrochemical analysis we can see that with the testing time going on, the corrosion potential, impedance arc radius, polarization resistance and corrosion current density of the steels show an increasing trend, which indicates the formation and thicken of rust layer could improve the corrosion resistance of steels, and the corrosion resistance of A plate and its rust layer is better than the other two.

**Keywords:** ship plate steel; simulated marine environment; cyclic immersion corrosion; atmospheric corrosion.

Poster Session 1

| P-A0069 |

# MIcrostructure control and stenghtening-toughening mechanism of 68.4GPa·% grade cold rolled steel

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## Abstract

A kind of medium manganese steel composed of Fe-6Mn-4Al-0.4C was designed. The effects of annealing parameters (temperature and time) on the microstructure evolution and mechanical properties after cold rolling were studied. With the increasing of annealing temperature , the yield strength decreased, the tensile strength first decreased and then increased, and the elongation first increased and then decreased. The mechanical properties change little with the increase of annealing time. The optimal heat treatment parameter of the steel after cold rolling is to hold the annealing temperature at 760°C for 30min, and then air cooling to room temperature. The tensile strength of the hot rolled specimens is 934MPa, the yield strength is 724MPa, the elongation is 73.3%, and the PSE reaches the highest value of 68.4GPa·%.

The microstructure evolution of the experimental steel mainly follows: carbide precipitation and redissolution, the formation of lamellar and equiaxed austenite and ferrite biphase structure. Lamellar grain transform into equiaxed grain, grain size coarse, austenite content increases, but transform into martensite due to the lack of stability. During the annealing process, the ferrite recrystallization occurs rapidly, accompanied by the reverse austenite transformation, and the final microstructure changes to equiaxed morphology.

The stability gradient of austenite in annealed specimens causes discontinuous TRIP effect. Ferrite deformation, dislocation density and austenite stability affect work hardening behavior. The volume fraction and stability of austenite play an important role in the comprehensive mechanical properties.

**Keywords:** Fe-6Mn-4Al-0.4C steel, Intercritical annealing, Microstructure control, Strengthening-toughening mechanism

| P-A0497 |

# Effects of Stress Triaxiality Distribution on Tensile Fracture of Notched TWIP Steel Plate

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## Abstract

The influence of stress triaxiality on the tensile-fracture of the TWIP steel plate was studied by conducting a series of tensile tests on smooth and notched specimens with different notch geometries. The stress triaxiality of the smooth specimen of ~0.33 remained unchanged to fracture. The overall fracture surface of the smooth specimen was macroscopically uniform and consisted of fine dimples regardless of the location. As the initial notch radius decreased (i.e., the initial stress triaxiality at the notch center increased), ductility remarkably decreased, but there was little change in the strength and reduction of area. The stress triaxiality of the notched specimens decreased continuously during the entire deformation. The fracture surface of the notch center of the notched specimens was covered with upstanding dimples. By contrast, the fracture surface of the notch edges consisted of severely sheared dimples, and the severity of shear became pronounced as the stress triaxiality gradient increased along the notch width. Even quasi-cleavage facets were dominantly observed at the notch edges with the higher stress triaxiality gradient. These results inform that the stress triaxiality gradient is an important factor determining the fracture mode of TWIP steel in addition to the local value of the stress triaxiality and imposed strain.

**Keywords:** TWIP steel, Tensile fracture; Stress triaxiality; Fractography; Digital image correlation

Selected Session: Advanced Steels and Properties

| P-A0732 |

# Integrated decarburization and oxidation model for high carbon-chromium containing steel

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## Abstract

The demand for High carbon-chromium-containing steels is consistently increasing in the automotive and structural sectors due to their desirable properties like high strength, superior wear resistance, extreme hardness, and moderate ductility. High C-Cr steel sheets are manufactured via a hot-strip rolling process where the rolled sheets are coiled at the down-coiler at around 600 °C and cooled in an atmospheric environment. Different amounts of air get trapped between the gap of the coil, and the volume of trapped air and the refresh rate of the draft depends on the coil's position and the windings' tightness. Due to this phenomenon, sheet metal at different coil positions gets subjected to different cooling and oxygen partial pressure conditions. The iron base and other alloying elements, such as carbon, chromium, silicon, and manganese, react with oxygen in the trapped air. As a result, external oxidation, decarburization, and internal oxidation co-occur on the sheet surface, which is detrimental to the finished product's quality. The rate of simultaneous occurring processes is assumed to be diffusion controlled. A combined thermodynamic and kinetic approach is used to model the oxidation-decarburization process and the changing gaseous environment. This work will discuss the comparison of model results with experimental data at 700 °C and 650 °C for representative alloys at atmospheric and lower oxygen partial pressures.

**Keywords:** High carbon-chromium steels, decarburization, oxidation, atmosphere control, Kinetic modeling

| P-A0971 |

# Hydrogen embrittlement of 300-series stainless steels under cryogenic conditions

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## Abstract

Eco-friendly liquid hydrogen(LH2) energy has gained significant attention in light of the impending carbon-neutral society. As a result, the significance of storage and transportation techniques, especially when it comes to selecting metallic materials for LH2 containers, has grown. Given the low boiling temperature of -253 °C, the careful choice of materials with favorable cryogenic properties becomes crucial for ensuring the safe handling of LH2 containers. Additionally, even a small amount of hydrogen gas can induce hydrogen embrittlement in metals. Consequently, the materials used for LH2 container should exhibit considerable resistance to both low temperature and hydrogen embrittlement.

Austenitic 300-series stainless steels have been suggested as candidate materials for LH2 storage tanks, because they show exceptional low-temperature mechanical properties and high resistance against hydrogen embrittlement due to the low diffusivity of hydrogen atoms in FCC structure. Nevertheless, there exists a limited number of studies investigating hydrogen embrittlement at cryogenic temperatures. This work aims to analyze hydrogen embrittlement mechanisms of 300-series stainless steels under cryogenic conditions, employing various perspectives.

**Keywords:** Cryogenic material, stainless steel, hydrogen embrittlement

| P-A0973 |

# Designing lightweight Co-free maraging steels

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## Abstract

Maraging steels have been extensively used in the industry needed high strength materials such as aerospace technology and military industry. The corresponding steels generally contain a large amount of Ni (17-19 wt.%), Co (8-12 wt.%), Ti (0.2-1.6 wt.%), Mo (3-5 wt.%), and a small amount of C (< 0.03 wt.%). After hot rolling and subsequent aging, the steels reveal the α′ martensitic matrix with intermetallic nanoprecipitates such as s Ni3Mo (D0a-type), Ni3Ti (D024-type), Ni3Al (L12-type), and Fe2Mo (C14-type), resulting in a high yield strength of over 1.4 GPa and a high tensile strength of over 1.6 GPa. However, despite its remarkable mechanical properties, the relatively high materials cost of the steel driven by expensive alloying elements hinders the mass production. Therefore, in the present study, we suggested the new alloy design concept of maraging steel with the merit of materials cost, and the microstructural evolutions and mechanical properties of the corresponding alloy are systematically investigated. Regarding the alloy composition, we used the Mn instead to reduce the Ni contents, also used the Al for low density and intermetallic precipitation. Additionally, we added the small amount of Cu for strengthening by nanoscale Cu precipitate and compared the Cu-free maraging steel with Cu-added maraging steel in present study.

**Keywords:** Maraging steel; Intermetallic precipitate; High-strength; Lightweight; Retained austenite

| P-A0980 |

# The relationship between thickness depth and hydrogen embrittlement in pipeline steel

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## Abstract

With the escalating consumption of crude oil and gas, there is an increasing demand for large-diameter pipe steel to ensure efficient transportation. Research focused on steel with excellent resistance to hydrogen induced cracking (HIC), which occurs during the transport of crude oil and gas containing H2S, has gained significant attention. The commonly used large-diameter steel composition typically consists of Fe-~0.28C-~1.4Mn-(Nb+V+Ti = 0.15) (wt.%). The microstructure of these pipe steel, treated using thermomechanical controlled processing (TCMP), exhibits variations such as ferrite, pearlite, and bainite, depending on the process temperature.

Meanwhile, in the case of thick pipeline steel plates, the microstructures of the steels could be varied toward thickness direction owing to the difference in cooling rates. These microstructural differences may lead to different mechanical properties. Therefore, this study aimed to investigate the microstructural changes toward thickness direction of thick pipeline steel plates, and discover the relationship between hydrogen embrittlement and microstructures.

**Keywords:** Pipeline steel, Thickness, Cooling rate, Microstructural imbalance, Hydrogen embrittlement

| P-A1003 |

# Comparison of Microstructural and Mechanical properties of Weld Joints in 9% Ni steel Prepared with Ni-based and Fe-based Filler Materials

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## Abstract

Welding is essential for fabricating the inner wall of LNG tanks using 9% Ni steel, which exhibits superior mechanical properties at both room temperature and cryogenic temperature. Ni-based filler materials, which form microstructure of FCC matrix and precipitations, have been applied for the welding of 9% Ni steel. A Fe-based filler material was developed to enhance the cost-effectiveness of filler material. The Fe-based filler material of controlled martensite-forming temperature forms a unique microstructure of austenite-covered packet lath martensite. A comparative analysis was conducted on the tensile properties of weld joints of 9% Ni steel using Ni-based and Fe-based filler materials at room and cryogenic temperature. In this study, we discussed the application of Ni-based and Fe-based filler materials for welding 9% Ni steel and conducted a comparison of the microstructure and mechanical properties of the weld joints.

**Keywords**: 9% Ni steel, Filler material, Mechanical properties, Cryogenic temperature

# POSTER Session 1

## Symposium B : Advanced Processing of Materials

**P-B0145** **A Study for effect of the void shape to material properties of plastic material with representative volume element**
YOUNGHYUN KIM (Korea Institute of Industrial Technology, Korea)

**P-B0223** **Microstructure and Mechanical Properties of Zinc Alloy Sheets Severely Deformed by ARB**
Ryuto Morinaga (Kumamoto University, Japan)

**P-B0277** **Systematic simulations of semi-solid deformation using multi-phase-field lattice Boltzmann method**
Namito Yamanaka (Kyoto Institute of Technology, Japan)

**P-B0283** **Solid-state diffusion bonding between CoCrNi-based high entropy alloys system and 316 stainless steel by spark plasma sintering**
HAOTIAN SUN (Hokkaido University, Japan)

**P-B0339** **Effect of impurity Zr contamination on properties of Ru-Mo-W alloys grown by the dewetting micro-pulling-down method**
Kotaro Yonemura (Tohoku University, Japan)

**P-B0371** **Effects of Heat Treatment in Hydrogen Environment on Hydrogen Permeability of Pd-40mass%Cu Alloy Membrane**
Hiroshi Yukawa (Nagoya University, Japan)

**P-B0705** **Interfacial analysis using Smoothed Particle Hydrodynamics (SPH) and Molecular Dynamics (MD) during Al-Fe High-Speed Vaporising Foil Actuator Welding (VFAW)**
DEEPAK KUMAR (INCHEON NATIONAL UNIVERSITY, INCHEON, REPUBLIC OF KOREA, Korea)

**P-B0730** **Characterization of AlSi10 Alloy Powder for the DED Process**
SUNGJAE JO (Kongju National University, Korea)

| P-B0145 |

# A Study for effect of the void shape to material properties of plastic material with representative volume element

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## Abstract

Due to climate change, carbon neutrality is receiving attention, and high-carbon industries are accelerating facility development for energy efficiency. The demand for factory automation using gantry robots is increasing, and cable chains for protecting cables during gantry robot movement are ultimately considered a key technological element for production efficiency and carbon neutrality in the process. In this study, the influence of the shape of internal voids in plastic materials on material quality was analysed using the homogenization method, with a focus on the most widely used representative volume element. In particular, the material properties were derived in different directions by analysing the material properties based on the size of the parameters that make up ellipsoidal voids. The use of an orthotropic matrix in this process, integrated with an FE simulation tool, not only enhances the reliability of the research but also ensures that the data is structured for practical field applications. This study analysed the impact of void shape on the quality of plastic materials and is applicable in practical setting.

**Keywords:** RVE, plastic, void, homogenization method, material properties

| P-B0223 |

# Microstructure and Mechanical Properties of Zinc Alloy Sheets Severely Deformed by ARB

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## Abstract

Accumulative roll-bonding (ARB), a typical severe plastic deformation, improves strength of metallic materials due to ultra-grain refinement. In this study, ARB was applied to ZDC2, commercially die-casting zinc alloys, at 283 K and 373 K, and the microstructure and mechanical properties were investigated. The grain refinement decreased and then saturated at 3-cycle of ARB at both temperatures; the mean grain size at 283 K was smaller than that at 373 K. Fractions of high-angle grain boundaries in ZDC2 deformed by ARB at 283K were also smaller than those at 373 K. Thus, dynamic recrystallization occurred more frequently at 383K. Grain growth has been reported to be suppressed by oxides at bonding interfaces in pure zinc deformed by ARB at 373 K. However, equiaxed grains were observed, but not bonding interfaces in ZDC2 deformed by ARB. Therefore, the effect of the bonding interface on grain refinement would be small in ZDC2. Texture of ZDC2 was found to differ from that of pure Zn after ARB. 0.2% proof stress increased with increasing ARB cycles at 373 K. On the other hand, 0.2% proof stress decreased after 3 cycles of ARB, and then saturated at 283 K. The difference was caused by different Schmid factors for basal slips against loading axis. Texture formation was found to be more effective to improve 0.2% proof stress in ZDC2, rather than grain refinement.

**Keywords:** ZDC2, grain refinement, texture, dynamic recrystallization, Schmid factor

| P-B0277 |

# Systematic simulations of semi-solid deformation using multi-phase-field lattice Boltzmann method

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## Abstract

During the casting process, semi-solid deformation due to external forces induces grain rearrangement. As a result, localized regions with low solid fraction are formed. These regions have a direct impact on macrosegregation or band segregation. Therefore, understanding the semi-solid deformation behaviour is crucial.

According to experiments, semi-solid deformation significantly differs depending on the solid fraction and grain morphology. Moreover, a thin semi-solid material was observed in situ, and it was confirmed that local dilatancy caused by grain–grain contact and rearrangement results in changes in the local solid fraction of the semi-solid material.

Numerical simulations were performed using discrete element method to gain a more detailed understanding of semi-solid deformation. It has been demonstrated through simulations that the solid fraction, grain morphology, and deformation rate have a significant impact on semi-solid deformation behaviour. However, these simulations were limited to semi-solid deformation with grains of artificial morphology.

In a previous study, we successfully simulated semi-solid deformation using the multi-phase-field lattice Boltzmann method and performed a continuous simulation from polycrystalline solidification to semi-solid deformation [Comput. Mater. Sci. 197 (2021) 110658]. In this study, systematic simulations were performed to assess the effect of solid fraction and crystal morphology on the transition of local solid fraction and to, thus, quantify the semi-solid deformation.

**Keywords:** Semi-solid deformation, Grain rearrangement, Solidification, Multi-phase-field method, Lattice Boltzmann method.

| P-B0283 |

# Solid-state diffusion bonding between CoCrNi-based high entropy alloys system and 316 stainless steel by spark plasma sintering

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## Abstract

Spark plasma sintering (SPS) is a new method for diffusion bonding of dissimilar metals. In this study, CoCrNi-based high entropy alloys (HEAs) system (CoCrFeNiMn, CoCrFeNi, and CoCrNi) were successfully joined to 316 stainless steels by SPS diffusion bonding, and the effect of bonding temperature and concentration on diffusion behavior and tensile property of bonded joints were investigated. The tensile strength of the HEAs/316SS joints were gradually increased with increasing bonding temperature. In addition, the tensile strength of the joints bonded at 0.8Tm were all exceeded 80% of that in 316SS. Meanwhile, the bonding at 0.8Tm had sufficient diffusion, resulted in the disappearance of voids and the increase in strength of joint. In CoCrNi/316SS joint, large element concentration variation would amplitude in the diffusion zone, could result in rapid diffusion of atoms and large diffusion distance. Furthermore, it suggests that the continuous FCC solid solution structure was generated in the diffusion zone, which was beneficial to the increase of tensile property in joints. The tensile strength and elongation of diffusion bonded HEAs/316SS joints were increased compared to laser beam welded joints. This study provides a feasible pathway for the application of diffusion bonding in HEAs, which could significantly broaden the application area of HEAs.

**Keywords:** Diffusion bonding; High entropy alloy; Medium entropy alloy; Composites; Diffusion behavior.

# Effect of impurity Zr contamination on properties of Ru-Mo-W alloys grown by the dewetting micro-pulling-down method

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## Abstract

High-temperature alloy wires have been used for the heaters of the vacuum evaporation method used to produce organic electroluminescent thin films. In conventional Ta wires, the formation of bamboo structures due to abnormal grain growth degrades the electrical and mechanical properties. Recently, we have developed Ru-Mo-W alloy (Ruscaloy) wires by the dewetting micro-pulling-down (μ-PD) method, which is a rapid single crystal growth method [1]. Ruscaloy wires have a lifetime approximately three times longer than that of Ta at 1873 K and higher electrical resistivity and toughness. However, the effect of impurity contamination to adjust the recycling concentration has not been studied. In this study, we investigated the acceptable impurity concentration of Zr in terms of electrical and mechanical properties and crystal growth.

Zr-doped Ru-Mo-W alloys were synthesized using an arc melting furnace with the raw materials of >99.9% purity. Single crystal wires with lengths of 11.8, 8.68, and 4.03 m were grown for Ru60Mo15W25 alloys with Zr additions of 0.1at%, 0.5at% and 1.0at%, respectively (Fig. 1). The diameters of the wires were 0.8 mm. After the annealing at 2273 K for 3 hours in high purity Ar atmosphere, the microstructure was observed, and the crystal orientation, tensile strength, and electrical resistivity were measured. The electrical resistivity increased with Zr addition (Fig.2). The details of the mechanical properties and behaviors in the crystal growth will be discussed.



**Fig.1** The grown wire of Zr 0.5 at% doped Ru60Mo15W25

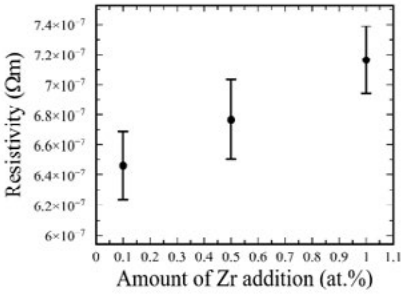



**Fig.2** Resistivity of the Zr doped Ru60Mo15W25

**Keywords:** Ru alloy, single crystal growth, refractory alloy, Resistance heating element

[1] R. Murakami, A. Yoshikawa et al., Int. J. Refract. Met. Hard Mater. (2023) In Press.

| P-B0371 |

# Effects of Heat Treatment in Hydrogen Environment on Hydrogen Permeability of Pd-40mass%Cu Alloy Membrane

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## Abstract

Pd-40 mass% Cu alloy membranes with a B2 crystal structure are in practical use as hydrogen-permeable membranes for hydrogen separation and purification, yielding ultra-high purity hydrogen. The typical operating temperature of this alloy membrane is around 623-723 K, but due to the low activation energy of hydrogen permeation, the alloy is expected to exhibit a relatively high hydrogen permeation capacity even at low temperatures below 473 K. However, hydrogen permeability performance at low temperatures has not been fully investigated. Previous studies have shown that the temperature dependence of hydrogen permeability exhibits a linear relationship following the Arrhenius equation at temperatures above 473 K. Below 473 K; however, the linear relationship deviates, and a significant decrease in permeability is observed, especially near room temperature, which is probably because defects in the material trap hydrogen at low temperatures.

On the other hand, the crystal structure of Pd-40 mass% Cu alloy after melt and rolling is an FCC (face-centered cubic) phase, so heat treatment is required for B2 transformation. This heat treatment is conventionally performed in a reducing hydrogen atmosphere, but the effect of the hydrogen during heat treatment on the hydrogen permeability of Pd-40 mass% Cu alloy is unknown.

In this study, Pd-40 mass% Cu alloy films with an FCC phase were heat-treated in different hydrogen pressure environments to investigate the effect of the hydrogen atmosphere during heat treatment on hydrogen permeability. As a result, the hydrogen permeability of the films annealed in hydrogen above 400 kPa was reduced compared to those annealed in hydrogen below 300 kPa. Also, the diffraction peaks of the samples annealed above 400 kPa were shifted to the higher angle side, indicating lattice contraction. These results suggest that hydrogen-induced vacancies are generated during heat treatment in a high-pressure hydrogen atmosphere.

**Keywords:** PdCu alloy membrane, CsCl-type crystal structure hydrogen permeability, hydrogen diffusivity, hydrogen trapping

| P-B0705 |

# Interfacial analysis using Smoothed Particle Hydrodynamics (SPH) and Molecular Dynamics (MD) during Al-Fe High-Speed Vaporising Foil Actuator Welding (VFAW)

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## Abstract

Interfacial analysis for impact welding methods is crucial for understanding the bond formation and optimising welding parameters. It provides insights into atomic-level interactions, diffusion, and material compatibility, enabling the development of advanced techniques and ensuring quality control. These analysis enhances the efficiency and reliability of impact welding processes, making them versatile for various industries. The present work performs an interfacial analysis using Smoothed Particle Hydrodynamics (SPH) and Molecular Dynamics (MD) simulations for Al-Fe joint formation during Vaporising Foil Actuator Welding (VFAW), which is a novel high-speed impact welding process. SPH is a meshless Lagrangian method, while MD is a particle-based technique for modelling interatomic interactions. This combined SPH-MD approach presents a comprehensive framework for understanding the interfacial behavior during VFAW. SPH simulations capture the dynamic behaviour of the molten material, while MD simulations focus on atomic-scale interactions at the Al-Fe interface. Results show the formation of complex intermetallic compounds at the interface, with varying compositions and morphologies. Visualization of material flow and heat transfer is achieved through SPH, while MD provides atomic-level details of interfacial interactions. The insights gained from this study contribute to the optimisation of VFAW parameters and the development of novel welding techniques. Furthermore, the methodology demonstrated here can be extended to investigate interfacial phenomena in other materials and manufacturing processes, enhancing our understanding of interfacial dynamics in various engineering applications.

**Keywords:** Smoothed Particle Hydrodynamics (SPH), Molecular Dynamics (MD), VFAW, Impact Welding, Al-Fe .

| P-B0730 |

# Characterization of AlSi10 Alloy Powder for the DED Process

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## Abstract

Additive manufacturing techniques have a significant positive impact on various industry sectors. Directed energy deposition (DED) is often preferred over powder bed fusion processes (PBF) for producing large components. Al alloys possess excellent physical and mechanical properties, such as specific strength, corrosion resistance, and ductility. It is feasible to increase machine efficiency by using lightweight materials and to enable lightweight design by using DED with Al alloy powder. However, the inherent physical properties of Al alloys pose challenges in achieving low-defect additive manufacturing of high-strength Al alloy as built, including issues like porosity, lack of fusion, and cracking.

It has been noted that the surface oxidation layer of powder affects the thermal conductivity, and reflectivity, and changes the ideal process parameters in DED. The use of satellite powders can increase pore formation, while an appropriate particle size distribution contributes to improved mechanical properties. Thus, powder characteristics are a crucial role in achieving low-defect additive manufacturing. In this work, the control of the AlSi10 powder properties is used to analyze the impact of powder characteristics on the DED process. AlSi10 alloy powder is fabricated by gas atomization, which is analyzed through X-ray diffraction (XRD) for phase and texture assessment and scanning electron microscopy (SEM) for particle shape and microstructure analysis. Vickers hardness, powder particle size distribution, and flowability are also measured to evaluate powder characteristics.

**Keywords:** Gas Atomization, Al alloy powder, powder characterization, Directed Energy Deposition

# POSTER Session 1

## Symposium C : Structural Materials for High Temperature

**P-C0257** **High temperature fatigue behaviour of β-phase containing TiAl alloys fabricated by metal 3D printing**
Koki Tanaka (Osaka University, Japan)

**P-C0684** **A Study on the Effects of Milling Media Variations on Mechanical Alloying Behaviour in High-Energy Milling of Nb Powder**
Deokhyun Han (Institute for Advanced Engineering, Korea)

**P-C0722** **Enhanced fracture toughness of Mo-Si-B-La2O3 alloys for high-temperature structural materials**
Wonjune Choi (Arizona State University, USA)

**P-C0744** **Microsutructural evolution of Mo-Si-B alloy using Mo powder with homogeneously dispersed oxide nanoparticles synthesized by ultrasonic spray pyrolysis**
Woocheol Kim (Seoul National University of Science & Technology, Korea)

**P-C0806** **Syntesis of Nb-Based MAX Phase Using Intermetallic Compounds of Nb-Al**
Siyeon Kim (Seoul National University of Science and Technology, Korea)

| P-C0257 |

# High temperature fatigue behaviour of β-phase containing TiAl alloys fabricated by metal 3D printing

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## Abstract

β-phase containing TiAl alloys have received considerable attention for aircraft engine application due to their low density and excellent high temperature strength. However, the poor ductility and high reactivity of the alloys hinder their precise manufacturing. Electron beam powder bed fusion (EB-PBF) which is one of the additive manufacturing technologies has attracted much attention as a new manufacturing process for the alloys because of its high energy density, low residual stress and high process speed. In recent years, it was found that the alloys fabricated by EB-PBF exhibit excellent high temperature tensile strength, compared to Ti-48Al-2Cr-2Nb alloys fabricated by casting. However, high temperature fatigue properties of the alloys have not yet been investigated.

In this study, high temperature fatigue behaviour of β-phase containing TiAl alloys fabricated by EB-PBF was examined, focusing on the influence of the microstructure. The ultrafine α2/γ lamellar grains with a lamellar spacing of approximately 30 nm can be obtained in the rods prepared by EB-PBF. Additionally, the β/γ cell structure is formed at the lamellar grain boundaries through a discontinuous precipitation reaction. We found that the fatigue strength of the rods at 1023 K is higher than that of cast Ti-48Al-2Cr-2Nb alloys. This is because the fatigue crack propagation is obstructed by the β phase in the β/γ cell structure.

**Keywords:** Additive manufacturing, Electron beam powder bed fusion, β-phase containing TiAl alloys, Microstructure, Fatigue properties

| P-C0684 |

# A Study on the Effects of Milling Media Variations on Mechanical Alloying Behaviour in High-Energy Milling of Nb Powder

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## Abstract

With the growing demand for sustainable energy solutions, there is an increasing need for enhanced power generation capabilities, greater efficiency, and high reliability. Ni-based superalloys, currently used in turbine blades, are effective only up to about 1150° C, closely approaching their usability limit given their 1455° C melting point. This necessitates the development of superheat-resistant alloys capable of operating in extreme conditions of 1200 ° C or higher. Niobium (Nb), with its high melting point of 2475 ° C, has been identified as a promising base alloy for ultra-high temperature environments of around 1300 ° C. However, the application of Nb is complicated by its limited oxidation resistance and inherent brittleness at room temperature.

This study examines the variations in mechanical alloying behavior due to different milling media during the high-energy, planetary milling of Nb and Si powders. The investigation concurrently assesses the mechanical alloying behavior, which is influenced by both the variations in kinetic energy associated with different milling media and the differing surface properties of the milling media materials. Subsequent analysis of the milled powders is carried out using X-Ray Diffraction (XRD), Particle Size Analysis (PSA), and Scanning Electron Microscopy with Energy Dispersive Spectroscopy (SEM-EDS). The XRD analysis explores residual stress and the extent of grain size/alloying through peak broadening. Changes in powder particle size from the original powder are assessed through PSA, while SEM-EDS is used to inspect powder cross-sections for evidence of mechanical alloying.

**Keywords:** Milling Media, Planetary Milling, ZrO2, WC, Mechanical alloying.

| P-C0722 |

# Enhanced fracture toughness of Mo-Si-B-La2O3 alloys for high-temperature structural materials

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## Abstract

Refractory metals, which usually have high melting point (above 2000°C), have been studied as next-generation high-temperature materials. Among them, molybdenum (Mo) alloys are powerful candidates due to their various advantages. In particular, Mo-silicide alloys (or Mo-Si-B alloys) with small amounts of silicon and boron have been studied to substitute current superalloys because of their superior mechanical properties and improved oxidation resistance at elevated temperature. Recently, there have been several attempts to improve its properties by adding a 4th element (e.g., Zr, Y, Ti, and La) in Mo-Si-B alloys.

In this study, the Mo-Si-B alloys with La2O3 particle will be discussed in terms of synthesis method and their mechanical properties. The Mo-Si-B multi-shell structured powder was prepared by calcination of La(NO3)3·6H2O. We confirmed that this powder was composed of Mo and La2O3 particles in a shell and Mo-Si-B intermetallic compound phases (Mo5SiB2 and Mo3Si phases) in a core. The Mo-Si-B-La2O3 sintered bodies were fabricated via cold isostatic pressing (CIP) followed by pressureless sintering. The microstructures of these alloys were investigated via scanning and transmission electron microscopy (SEM and TEM, respectively) and electron back scattered diffraction (EBSD). The fracture toughness was measured using a three-point bending test, and Mo-Si-B alloy with 0.3 wt.% La2O3 particle showed an enhanced fracture toughness of 17.0 MPa·m1/2. Considering the microstructural analysis results, the improved fracture toughness is highly affected by the size and the distribution of the oxide particles (La2O3).

**Keywords:** Mo-Si-B alloys, High-temperature materials, Fracture toughness, Oxide dispersed strengthening (ODS), Lanthanum oxide (La2O3)

| P-C0744 |

# Microsutructural evolution of Mo-Si-B alloy using Mo powder with homogeneously dispersed oxide nanoparticles synthesized by ultrasonic spray pyrolysis

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## Abstract

High temperature materials are utilized in extremely harsh environments where temperatures and pressures are exceptionally high. Representatively, there are Ni–based superalloys applied to turbine blades. The temperature and pressure that high temperature materials must endure have increased recently. As a result, there are many attempts to find new material to replace Ni-based superalloys, and Mo–Si–B alloys are promising candidates for new high temperature materials.

The melting point of Mo-Si-B alloys is higher than that of the Ni-based superalloys, and they have excellent high temperature mechanical properties. Mo–Si–B alloys, in particular, composed of Mo phase and intermetallic compound phases have received special attention due to their remarkable properties including oxidation resistance and mechanical properties at high temperature. However, it has yet to be used to components due to the insufficient fracture toughness at room temperature. To address this problem, research is being conducted on Mo-Si-B alloys with dispersed oxides. Oxide dispersion strengthening is an effective strengthening mechanism in high temperature materials. Therefore, various attempts have been made to disperse oxides into particles, and Ultrasonic Spray Pyrolysis(USP), which can simply and uniformly disperse oxides of various compositions, is considered as an effective production method.

In this study, the effect of the dispersed oxide on the properties of the Mo-Si-B alloy was investigated by fabricating the Mo–Si–B alloy with oxide dispersed. Mo particles with uniformly dispersed oxides were prepared through USP, and Mo-Si-B alloys with uniformly dispersed oxides were prepared and analyzed through a mechanochemical method.

**Keywords:** High temperature material, Mo-Si-B alloy, USP, Dispersed oxide, mechanochemical process

| P-C0806 |

# Syntesis of Nb-Based MAX Phase Using Intermetallic Compounds of Nb-Al

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## Abstract

MAX Phases are gathering significant attention as materials for aerospace due to its high-temperature stability and chemical resistance. Also it can serve as a refractory material, and its exceptional thermal conductivity makes it suitable for implementation as a thermally conductive material. MAX Phase is represented as Mn+1AXn (n=1, 2, and 3), where M denotes a metallic element (Ti, Mo, Nb, etc.), A represents a group 3 or 6 elements (Al, Si, etc.), and X signifies a non-metallic element (C, Ni, etc.), forming layered structures. Among them, Nb-based MAX Phase exhibits superior properties such as high-temperature corrosion resistance and mechanical strength compared to other MAX Phase materials. However, when synthesizing Nb-MAX, using raw powders it becomes challenging to precisely control the elemental ratios, leading to the incomplete reaction between powders and difficulty in achieving the desired MAX Phase composition.

Therefore, we aimed to obtain Nb2AlC using intermetallic compounds of Nb-Al. To achieve this goal, Nb-Al intermetallic compounds were fabricated through ball milling. And differential scanning calorimetry(DSC) confirmed that Nb3Al exhibited the most pronounced exothermic reaction among the Nb-Al intermetallic compounds. Additionally, experiments were conducted to overcome the aluminum loss issue by adjusting the amount of Al, thereby determining the optimal aluminum content for Nb2AlC synthesis. As a result, Nb2AlC synthesis was successfully achieved at lower temperatures compared to conventional manufacturing processes, facilitating the easier production of Nb2AlC materials.

**Keywords:** Nb-based MAX Phase, intermetallic compounds, Aluminum content control

# POSTER Session 1

## Symposium D : Light Metals and Alloys

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# **POSTER** Session **1**

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**P-D0786** **Effects of rare earth addition on microstructure, mechanical properties, and electrical conductivity of Al-Mn-Cu-Fe-Si-Zn based alloy**
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| P-D0026 |

# Effect of La on Mechanical Properties and Precipitated Phase Stability of 2195 Al-Li Alloy at Elevated Temperature

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Key words: Aluminum lithium alloy; La; T1(Al2CuLi); θ′(Al2Cu); Heat exposure; mechanical properties.

## Abstract

This paper investigated the effect of La on the mechanical properties and precipitation phase stability of 2195 Al-Li alloy at an elevated temperature. After the different heat exposure experiments, the morphology of the precipitated phase and stability of tensile properties of the 2195 Al-Li alloy with the different ratios of La/Ag were analyzed by TEM and tensile properties test. The purpose is to investigate the method of preparing an aluminum alloy drill pipe that meets the use requirements of La instead of high-priced Ag. The experimental results show that the tensile strength of the 2195 alloy was prepared using 0.05wt% La instead of 0.2wt.% Ag at T6 peak age is the same as that of 2195 alloy containing 0.4% Ag, and its mechanical properties are stable after thermal exposure under different conditions. After heat exposure at 180 °C for 60 hours, the tensile strength of 2195 alloy containing 0.1wt% La but without Ag decreased by 42.2MPa, and its mechanical properties remained at a high level ($\sigma b \geq 530$MPa, $\sigma 0.2 \geq 480$MPa, $\delta \geq 7\%$). The above results provide a new idea for designing and preparing high-quality, low-cost aluminium alloy drill pipes.

| P-D0293 |

# Effect of microstructure on fatigue properties of Mg-Zn-Y and AZ31B

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## Abstract

Mg-Zn-Y alloys have two -phases: long-period stacking structure (LPSO) phases and α-Mg matrix phases. Moreover, the alloys had a multimodal microstructure consisting of recrystallized α-Mg grain regions, worked α-Mg grain regions, and LPSO phase regions. To investigate effects of the multimodal microstructure on fatigue properties, fatigue tests of extruded AZ31B, Mg99.2Zn0.2Y0.6 and Mg97Zn1Y2 alloys were carried out at room temperature. The extruded AZ31B consisted of two regions: recrystallized grain regions and worked grain regions Mg97Zn1Y2 and Mg99.2Zn0.2Y0.6 alloys had a multimodal microstructure with LPSO phases. The fatigue limit of all alloys was approximately 160MPa. However, the fatigue life of Mg-Zn-Y alloys was shorter than that of AZ31B at stress amplitudes of 180~200MPa. The crack growth rate in the recrystallized grain regions was slower than that in the worked grain regions in AZ31B. However, in Mg-Zn-Y alloy, the crack growth rate was independent of the multimodal microstructure, suggesting almost identical crack growth rates in both recrystallized and worked grain regions. In other words, the difference in fatigue life between AZ31B and Mg-Zn-Y can be attributed to the difference in crack growth rates in recrystallized grains and working grains depending on alloy composition.

**Keywords:** LPSO, multimodal microstructure, crack growth rate

| P-D0304 |

# Torque Characteristics and Cyclic Deformation Behaviour of Ti-Ni Superelastic Alloy Spiral Spring

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## Abstract

The objective of this study is to develop a new spiral spring that exhibits unique deformation behavior. The spiral spring is made of Ti-Ni superelastic alloy wire.

Currently, Ti-Ni superelastic alloys have considerable promise as materials of energy storage devices and actuators. However, Ti-Ni superelastic alloys are difficult to process, therefore there is little knowledge about energy storage properties.

In this study, we proposed the preparing method of Ti-Ni superelastic alloy spiral spring. In addition, the torque characteristics and cyclic deformation behavior of the spiral spring were investigated. In this study, the commercially available superelastic alloy wires (0.5 mm and 0.7 mm in diameter) were used to prepare spiral spring. Furthermore, torque characteristics measurement system was developed. The system can be monitored torque characteristics of spiral spring during wind and rewind process. Effects of cyclic deformation, i.e., repetition of wind and rewind process, on torque characteristics were evaluated.

Three main results were obtained. First, the torque characteristics of the Ti-Ni superelastic alloy spiral spring show a constant torque output. Therefore, the spiral spring is suitable for the energy storage device. Second, the torque characteristics change with the number of cyclic deformation tests. Third, although the magnitude of torque changes depending on the thickness of the spring material, there is no significant change in torque characteristics.

**Keywords:** Superelastic alloy, Ti-Ni, spiral spring, Torque characteristics, Energy storage

Poster Session 1

| P-D0305 |

# Hydrogen embrittlement behavior of 7xxx aluminum alloys processed by sliding friction treatment and subsequent aging

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## Abstract

7xxx aluminium alloys show high strength due to precipitation hardening, however, they are susceptible to hydrogen embrittlement based on intergranular cracking. We need to develop the thermo-mechanical treatment to supress hydrogen embrittlement. In this study, effect of sliding friction(SFT) and subsequent aging on hydrogen embrittlement behavior of 7xxx alloys was investigated. Cold-rolled specimens were solution-treated, water-quenched and followed by SFT. SFT resulted in grain refinement and increasing of hardness near the specimen surface. Hydrogen embrittlement sensitivity(HES) was evaluated by means of a slow strain rate technique tensile test in two environments, humid air(HA) and dry nitrogen gas(DNG). The T6 -tempered and SFT + aged specimens were examined. The T6-tempered specimens showed a loss of elongation in HA compared to in DNG based on intergranular cracking. The area fraction of intergranular cracking in SFT + aged specimen was smaller than in T6-tempered specimen. Therefore, the surface deformed layer introduced by SFT was effective to suppress hydrogen-induced grain boundary cracking of 7xxx alloys in humid air.

**Keywords:** Al-Zn-Mg alloy, hydrogen embrittlement, humid air, slow strain rate technique, sliding friction treatment

| P-D0312 |

# Effects of nitrogen content on microstructural stability and mechanical properties of fine-grained Ti-N alloy

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## Abstract

Titanium and its alloys exhibit high specific strength and excellent corrosion resistance. Adding interstitial atoms to Ti, especially nitrogen atoms, is expected to furthermore increase the strength. Moreover, the addition of nitrogen would also significantly reduce the grain growth rate of Ti-N alloys. In this study, we aim to systematically investigate recrystallization behavior of Ti-N alloys with different nitrogen contents and to clarify the effect of nitrogen content on mechanical properties of the Ti-N alloys having fine-grained fully recrystallized microstructures. By high-pressure torsion (HPT) and subsequent annealing, we could obtain fully recrystallized Ti-xN (x=0, 0.3, 0.6 wt.%) alloys with different average grain sizes (D). It was found that the grain growth rate decreased significantly with increasing the nitrogen content. It was also confirmed that recrystallization texture changed depending on the nitrogen content. Tensile tests were conducted at room temperature to evaluate mechanical properties of these specimens. The results showed that the fine-grained (D=3.6 μm) Ti-0.3N alloy exhibited a yield strength 5.2 times higher than that of pure Ti while maintaining a reasonable uniform elongation. In contrast, the Ti-0.6N alloy showed brittle fracture in elastic range, regardless of the grain size.

**Keywords:** titanium, Ti-N alloy, mechanical property, recrystallization, microstructure

| P-D0386 |

# Characteristics of Phosphate Film Formed on Cavitation-Treated AZ31 Magnesium Alloy Surface in Water

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## Abstract

Cavitation processing with chemicals was used to improve the corrosion resistance of an AZ31magnesium alloy surface. This technique improves corrosion resistance by the formation of a phosphoric acid film on the surface of the Mg alloy. However, the processing conditions affect the state of the film; therefore, the effect of the distance from the nozzle to the specimen surface (stand-off distance) on the cavitation state was investigated. Since this technique employs phosphoric acid and water for processing, immersion tests were performed with various aqueous concentrations of phosphoric acid. Cavitation processing uses water jet peening (WJP) and multifunction cavitation (MFC). The stand-off distance at which the phosphoric acid-based film was easily formed on the Mg alloy surface was specified for each processing condition. In the immersion test, metallic luster colors were observed on the surface after immersion with phosphoric acid concentrations of 0.002 and 0.001 mass%, golden colors were observed at 0.01 and 0.2 mass%, and black color was observed at 0.1 mass%. The surface color was uneven except for the surface processed at a phosphoric acid concentration of 0.1 mass%.

**Keywords:** Multifunction cavitation, Residual stress, Hardness, water jet peening, Immersion test

Poster Session 1

| P-D0552 |

# Microstructure observation of Mg-Zn-Al alloy aged at 423K

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Magnesium (Mg) has been widely used as structural materials, for example, electrical devices, frame of automobile parts due to its light weight. Several reports are available about precipitation hardening of Mg-Zn alloys. Recent studied suggested the precipitation sequence of Mg-Zn alloy like: S.S.S.S. → G.P. zone → β1'(MgZn2 and Mg4Zn7)→ β2'(MgZn2) → β(MgZn). However, nucleation sequence, crystal structure and orientation relationship with matrix are not clearly revealed yet. In this study, Mg-2.2mol%Zn (2Zn) and Mg-2.2mol%Zn-0.8mol%Al (2ZA) were prepared by gravity casting. Both alloys were homogenized at 593K for 12h and rolled to 1mm for 3mm thickness. Then, samples were subjected to solution treated at 603K for 1h using a quartz tube with argon atmosphere and quenched in water at 293K. Aging process were conducted by using oil bath at 423K. Mechanical property was investigated using Vickers microhardness measurement. Microstructure observation was conducted using TEM (transmission electron microscopy, TOPCON 002B) under accelerated voltage of 120 kV. Thin foils were prepared by twin-jet electron polishing using a solution of nitro acid: phosphoric acid: methanol = 1.5: 1.5: 7.0. 2ZA alloy showed higher the number of precipitation density than 2Zn. It is responsible for the higher hardness level of 2ZA.

**Keywords:** Mg-Zn-Al alloy, aging hardening, TEM, precipitate

| P-D0560 |

# Optimizing the microstructures and enhancing the mechanical properties of AZ81 alloy by adding TC4 particles

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## Abstract

In this work, AZ81 alloys reinforced with 3 wt.%, 6 wt.% and 9 wt.% TC4 (Ti-6Al-4V) particles were fabricated using two-step stirring. The tensile results revealed that the TC4 particles could significantly improve the yield stress (YS), ultimate tensile stress (UTS), and elongation (El.) of AZ81 alloys. By adding TC4, the grains showed refined/coarse bimodal morphologies in the composites. The formation of β (Mg17Al12) phase was notably suppressed due to the interfacial reaction between TC4 and Al. The dynamic recrystallization (DRX) behavior was also restricted by TC4 particles and β phase, ascribing to the refined grains and Orowan strengthening. The good interfacial bonding was achieved at the interface of TC4/α-Mg in 6TC4/AZ81 composite. Compared to the AZ81, 6TC4/AZ81 showed the highest YS, UTS and El. of 241 MPa, 357 MPa, and 17.0%, respectively. Its increased strength was primarily attributed to the mismatch coefficient of thermal expansion (CTE) and grain boundary strengthening. The improved ductility was ascribed to the TC4 particles, which are more deformable to withstand external load.

**Key words:** Mg alloy, TC4 particles, mechanical properties, strengthening mechanism

| P-D0667 |

# Effect of cold rolling and annealing conditions on stretcher strain marks in new high Mg-added Al-Mg alloys

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## Abstract

The exceptional combination of strength, formability, and corrosion resistance exhibited by the Aluminium 5xxx series alloys has made them widely used in diverse industries. These alloys provide versatile solutions for a variety of applications that demand reliability and high performance. However, increasing the strength of these alloys while maintaining or enhancing their ductility could expand their further potential applications. One approach to achieve this is by developing new Al-Mg-based alloys with higher Mg contents, as it offers excellent strength and ductility. However, previous research has shown that increasing the Mg content in Aluminium 5xxx series alloys leads to a significant increase in stretcher strain marks (SSMs), which affects the mechanical properties and surface appearance, and exhibits anisotropic behaviour. Therefore, the objective of this study was to investigate the effect of cold rolling and annealing conditions on SSMs, tensile strength, and ductility. In the experimental process, we used three kinds of Al-Mg alloys containing 6, 8, and 8.5 mass % of Mg contents. These alloys were fabricated by alloying Mg in the form of Mg+Al2Ca master alloy (also known as Eco-Al processing) to protect the melt of these high Mg-added Al-Mg alloys. The as-cast alloys were then subjected to hot rolling followed by cold rolling. The microstructure was observed at various stages such as the as-cast billet stage, after hot rolling (90 % thickness reduction), after cold rolling (75 % thickness reduction), and after the annealing stage (partial and fully annealed). Stretcher strain marks have been observed using the Digital Image Correlation (DIC) technology (GOM Snap 2D 2020 Software).

**Keywords:** Al-Mg alloys, high Mg contents, microstructure, Stretcher Strain Marks, DIC.

| P-D0680 |

# Influence of Al content change on microstructure and mechanical properties of Mg-Li alloy

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## Abstract

Magnesium alloy, the lightest metal structural material, can be applied to many fields such as the aerospace industry and electronic parts materials. However, magnesium alloys have a disadvantage in that formability is poor at room temperature due to the crystal structure of close-packed hexagonal crystals (HCP). An alloy that can compensate for these disadvantages is a magnesium-lithium alloy. When lithium is added to the magnesium alloy, α-Mg (HCP) occurs when the lithium content is less than 5.7 wt.%, α (HCP) + β (BCC) when the lithium content is between 5.7 and 10.3 wt.%, and β- when the content is 10.7 wt.% or more. It has a structure of Li (BCC) and can be molded at room temperature. Also, by adding lithium (0.534 g/cm3), which has a lower density than magnesium (1.738 g/cm3), it is possible to develop an ultralight alloy with a lower density. In this study, a study was conducted on the microstructure and mechanical properties of Mg-8Li-0.5Zn alloy with 4, 6, and 8 wt.% of Al. Each alloy was prepared by gravity casting in an SF6+CO2 gas atmosphere using an electric furnace, and a 12mm plate-shaped extruded material was produced at an extrusion ratio of 7.4:1 through direct extrusion. Through cold rolling, a 7mm plate was manufactured from a 12mm extruded material at a reduction rate of 58.3%. FE-SEM and EBSD were used to analyze the microstructure of each alloy, and tensile tests were performed on extruded and rolled materials to evaluate mechanical properties.

**Keywords:** magnesium, lithium, aluminum, microstructure, mechanical properties

| P-D0687 |

# Study on properties and precipitation behavior of Al-Mg-Si alloys with trace In content

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## Abstract

Al-Mg-Si alloys are widely used in high temperature pistons and battery housings for eco-friendly vehicles because of their excellent strength, good electrical conductivity, and low masses. The mechanical properties of Al-Mg-Si alloys are controlled by age hardening w due to forming masses of nanosized precipitates during aging. However, the nanosized precipitates in the Al-Mg-Si alloys are inevitably coarsened when the alloys are exposed to thermal environment, triggering a deterioration of mechanical properties. Microalloying is one of the most efficient ways to prevent thermal deterioration by regulating the vacancy diffusion during aging or segregation into interface of matrix-precipitate. Among them, In is a prominent microalloying element because it shows a strong interaction with vacancies, has a relatively high solubility in the α-Mg matrix, and can be segregated into matrix-precipitate interface. In this work, the precipitation behavior of Al-Mg-Si ternary alloys with various Mg/Si ratios from 0.5 to 2.0 and trace In addition (0.2 wt.%) under various aging conditions was systematically studied by microhardness measurements, atom probe tomography (APT), high angle annular dark field scanning transmission electron microscopy (HAADF-STEM). The individual and collaborative effects of In addition and Mg/Si ratio on the microstructure evolution, mechanical properties, and thermal stability were investigated in this study. The cluster and precipitate characteristics such as type, volume fraction, and size distribution were detailed and used to estimate the contribution to material strength. It is expected that the results of this study are beneficial for the production of Al–Mg–Si series alloys.

**Keywords:** Al-Mg-Si alloy, Precipitation strengthening, Microstructure, Property, Nano-cluster

| P-D0773 |

# Cryogenic Temperature Toughness of binary Al-Mg Alloys using Charpy impact tests

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## Abstract

In this study, the Mg and temperature effects on cryogenic impact toughness of Al-Mg alloys are investigated. Cryogenic Charpy impact tests are conducted for several Al-Mg alloys: AA5083 (= reference), Al-6Mg, Al-8Mg, and Al-8.5Mg. The temperature range is – 196 ˚C to 100 ˚C. In all Al-Mg alloys, the impact toughness is improved at higher temperatures. The Al-6Mg alloy exhibits the largest impact toughness, whereas the lowest impact toughness is observed in AA5083 over the temperature range. Beyond the Mg content of 6 wt%, the impact toughness of Al-Mg alloys decreases with increasing Mg. The planar anisotropy (Δr) is low in Al-Mg alloys of higher impact toughness. The largest amounts of coarse inclusions (> 10 μm) are present in the AA5083, providing favorable cracking sites and thereby its poor impact toughness. The grain size and intergranular Mg segregation do not appear to influence the toughness of Al-Mg alloys. Weaker texture in the most ductile Al-6Mg appears beneficial to gain more homogeneous deformation and lower Δr. Brass {110}<112>, S {123}<634>, and Copper {112}<111> textures evolve at the expense of a Goss {110}<001> weakening by increasing the Mg level. This texture evolution illustrates the toughness degradation of Al-Mg alloys of higher Mg levels.

**Keywords:** Al-Mg alloys; cryogenic properties; impact toughness; microstructure; texture

Poster Session 1

| P-D0786 |

# Effects of rare earth addition on microstructure, mechanical properties, and electrical conductivity of Al-Mn-Cu-Fe-Si-Zn based alloy

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## Abstract

Aluminum alloys are widely applied in the power industry due to their excellent conductivity, low cost, good formability, corrosion resistance and low density. In the case of electrical products, if heat dissipation characteristics are not secured, efficiency and lifespan rapidly drop, so heat dissipation performance is required for high output. However, it is difficult to satisfy both high strength and high conductivity, and research on improving strength while minimizing the decrease in conductivity is required. Al-based immiscible system such as rare earth(RE) appears to be a promising material for high-conductance materials because of its negligible effect on the electrical conductivity since the solubility of the aluminum alloy is zero. In this study, changes in the microstructure, mechanical properties, and electrical conductivity of as-cast and as-extruded Al-Mn-Cu-Fe-Si-Zn based alloy with the addition of RE were investigated. The microstructures of the alloys were examined using a field emission scanning electron microscopy (FE-SEM) and electron backscatter diffraction (EBSD) system. The phase composition of the alloys was examined using a scanning electron microscope equipped with an energy-dispersive X-ray spectrometer (EDS). The electric conductivities of the alloys were measured using the eddy current method at room temperature. The mechanical properties of the as-extruded Al alloy specimens were measured by universal testing machine with ASTM E8M standard.

**Keywords:** Aluminum alloy, Rare earth, Microstructure, Mechanical properties

| P-D0847 |

# Effects of Superheating Treatment and T6 heat treatment on the tensile properties and thermal conductivity of Fe bearing Al-10Si-Mg casting alloy

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## Abstract

The effect of T6 heat treatment on Fe-bearing Al-10Si-0.35Mg alloy was investigated in this study. By superheating the alloy at 820°C for 1 hour, the size of Fe intermetallic compounds was controlled to enhance mechanical and thermal conductivity properties. Two alloy types of superheated-F and conventional-F were prepared and compared. Both alloys were conducted at solid solution treatment at 535°C for 1 hour, followed by T6 heat treatment at 190°C for 6 hours. The microstructure analysis showed a change in the morphology of eutectic Si from a coarse lamellar or acicular shape to a blocky shape, and the area fraction of eutectic Si and AlFeSi intermetallic compounds was measured as conventional-T6: 12.49%, 11.8%, and superheated-T6: 11.8%, 9.8% respectively. It is also confirmed that the Si particle size was refined by superheating treatment. TEM observations represented the precipitation of Mg2Si precipitates in the β″ phase after T6 heat treatment. Tensile tests were conducted at room temperature with a strain rate of 10-3/s. Conventional-T6 showed 240.2MPa (YS), 313.3MPa (UTS), and 8.1% (El.). Superheated-T6 showed 265.3MPa (YS), 340.3MPa (UTS), and 7.7% (El.), indicating improved mechanical properties by inducing superheating treatment. Furthermore, the thermal conductivity increased after superheating treatment, with conventional-T6 measuring 161.8W/m·K and superheated-T6 measuring 174.7W/m·K. Based on the aforementioned findings, this study also discussed the effect of superheating treatment and T6 heat treatment on the deformation behavior and the thermal conductivity mechanism of Fe-bearing Al-10Si-Mg casting alloy.

**Keywords:** Al-10Si-Mg, Fe-intermetallic compound, Tensile property, Thermal conductivity, T6 heat treatment

| P-D0874 |

# Applications of non-flammable and corrosion resistant Mg-Al-Zn-Mn-Ca-Y alloys

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## Abstract

Mg-Al-Zn-Mn-Ca-Y alloys with simultaneous improvement in non-flammability and mechanical properties of AZ-based alloys were developed by the Korea Institute of Materials Science. The effect of small addition of Ca and Y has resulted in a tremendous improvement in the properties of magnesium alloys such as non-flammability, corrosion resistance, room temperature formability. These Mg-Al-Zn-Mn-Ca-Y alloys are named as the SEN (Stainless, Environment, Non-flammable) alloys. The SEN alloys have various characteristics from SEN1 (Al: 1 wt.%) to SEN11 (Al: 11 wt.%) depending on the Al content. SEN1 to SEN3 are used for sheet products with excellent formability and corrosion resistance. SEN6 has superior corrosion resistance and can be used for a high-toughness wrought alloy for high-speed extrusion. SEN9~SEN11 alloys are used for aircraft or railway vehicles that require high strength. We are currently conducting prototype development and implementation research through the cooperation with many domestic and foreign magnesium manufacturers, which will be presented in this talk

**Keywords:** Non-flammability, Corrosion resistance, SEN, formability, diecasting

# POSTER Session 1

## Symposium E : Additive Manufacturing

**P-E0083** **Shear deformation behavior of additively manufactured 316L stainless steel lattice structures**
Gitaek Lee (Pohang University of Science And Technology, Korea)

**P-E0276** **Multi-phase-field modeling to compute material microstructure evolutions affected by liquid flows during powder bed fusion**
Konosuke Ikeda (Kyoto Institute of Technology, Japan)

**P-E0298** **Effect of Excess Vacancies Induced by Laser-Beam Irradiation for Additive Manufacturing on Growth of Antiphase Domains in Fe3Al Phase**
Tsubasa Sato (Osaka University, Japan)

**P-E0406** **Effect of process parameters on the mechanical properties of maraging steel(18Ni-300) manufactured by powder bed fusion**
Hyo-Kyu Kim (Korea Institute of Industrial Technology, Korea)

**P-E0590** **Effects on trace element and carbon on microstructure, mechanical properties and thermal conductivity of the 3D-printed Fe-Cu based alloy using by LPBF process**
Hyeon-Taek Son (Korea Institute of Industrial Technology, Korea)

**P-E0597** **Effect of Property Differences between Virgin and Used 18Ni300 maraging steel Powders on Mechanical Properties of Additive Manufacturing**
Joseph Jo (Korea University School, Korea)

**P-E0614** **Cubic and Epsilon Cobalt Phases in Direct Energy Deposition Additively Manufactured Co-Cr-W Alloy**
Jinsung JANG (Korea Atomic Energy Research Institute, Korea)

**P-E0649** **Study of tensile properties and microstructure according to process parameters of Fe-2.7Mn-6.0Al-0.4C lightweight steel manufactured using DED**
Kwang Kyu Ko (Gyeongsang National University, Korea)

**P-E0659** **Microstructure-Based Post-Heat Treatment Design of Inconel 939W fabricated by Laser-Powder Bed Fusion for Creep Enhancement**
CheolHyeok Yang (Changwon National University, Korea)

**P-E0697** **Understanding the superior mechanical properties of hollow-strut metal lattice materials**
Tingting Song (RMIT University, Australia)

**P-E0868** **Ultrastrong yet ductile additively manufactured steel via tailori tenite stability**
Jinhua Wang (Tsinghua University, China)

| P-E0083 |

# Shear deformation behavior of additively manufactured 316L stainless steel lattice structures

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## Abstract

Selective laser melting (SLM) and additive manufacturing (AM) techniques have recently attracted the substantial interest of both researchers and the processing industry. The ability to design freely has opened up new possibilities for structure and products. Despite its promising potential, there are still challenges to overcome, such as porosity, which will be examined closely in this study. The hot isostatic press (HIP) process significantly affects the microstructure of additively manufactured materials and can reduce internal defects and improve material properties. However, liquation cracking can occur in alloy 718 due to the Nb-rich Laves phase and carbide. This study compared the liquation cracking behavior of additively manufactured samples under three different heat treatment conditions (As-built, stress-relieved, and HIPed). The samples were subjected to a hot ductility test using a thermal-mechanical simulator (Gleeble 3500), and the nil ductility temperature (NDT) and ductility recovery temperature (DRT) were compared. The NDTs were similar in all cases, but the HIPed sample showed a lower DRT than the other two conditions. Coarsening of the grain size and NbC carbide were observed in the HIPed sample, which made the material more susceptible to liquation cracking due to the decrease in grain boundary length and growth of the Nb-rich phase.

**Keywords:** Additive manufacturing; Liquation Cracking; Thermal-Mechanical Simulator; High-Temperature Materials; Characterization

| P-E0276 |

# Multi-phase-field modeling to compute material microstructure evolutions affected by liquid flows during powder bed fusion

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## Abstract

Powder bed fusion (PBF), a typical technique in metal additive manufacturing (AM), involves complex multiphysics phenomena, such as laser irradiation on the powder particles and substrate; melting, solidification, and fluid flows in the molten pool; and polycrystalline grain growth after solidification. Generally, the solidification microstructures and defects formed during PBF, which play a critical role in determining the properties of AM products, is significantly influenced by the fluid flow within the molten pool. However, direct observations of such formation processes are not usually straightforward. Therefore, numerical simulations are essential for predicting such multiphysics phenomena. Several numerical simulation studies have explored PBF under various spatiotemporal scales. However, the accuracy of numerical methods has to be improved because the interface tracking models used for predicting material microstructures, such as cellular automaton and phase-field (PF) methods, and those used for predicting fluid flows, such as fluid volumes, are different.

Notably, the PF method can accurately reproduce material microstructure formation processes [Comp. Mater. Sci. 197 (2021) 110658] and multiphase flows [Comput Fluids, 178 (2019) 141–151]. Therefore, combining various PF methods developed across different fields may aid in accurately determining the multiphysics phenomena of PBF. In this study, we attempted to construct a numerical model capable of predicting solidification microstructures and defects affected by liquid flows in PBF. Particularly, we coupled a multi-phase-field (MPF) model to express material microstructure evolutions, such as melting, solidification, and grain growth, with a multiphase flow MPF model to solve liquid flow and keyhole formation in the melt pool. Using the developed numerical model, we performed two-dimensional laser scanning simulations and confirmed that it could represent the multiphysics phenomena in PBF.

**Keywords:** Phase-field method; Material microstructure; Multiphase flow; Powder bed fusion; Additive manufacturing

Poster Session 1

| P-E0298 |

# Effect of Excess Vacancies Induced by Laser-Beam Irradiation for Additive Manufacturing on Growth of Antiphase Domains in Fe3Al Phase

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## Abstract

Fe3Al intermetallic single crystals show pseudoelasticity by the interaction between antiphase domain boundaries and dislocations. Recently, additive manufacturing (AM) processes have attracted much attention because of the degrees of freedom in shapes. In addition, the laser powder-bed fusion (L-PBF) type AM process can fabricate single crystal parts by applying the narrow-pitch scanning strategy. If Fe3Al single crystals are fabricated by L-PBF, they will be useful in practical applications. However, the excess vacancies introduced by rapid cooling in the L-PBF process would affect the growth of APD, which is closely related to the mechanical properties of the fabricated single crystals. In this study, we investigated the growth of APD in the laser-irradiated regions of the Fe-28at.%Al alloy by transmission electron microscopy (TEM) to reveal the effect of excess vacancies on APD growth. Phase-field simulations are also performed to estimate the ordering mobility of the APD influenced by excess vacancy. It was found that the laser-irradiated and rapidly cooled regions show faster APD growth during ordering heat treatment than that in water-quenched regions. Excess vacancies introduced by the rapid cooling are suggested to promote the APD growth of the Fe3Al intermetallic phase. The ordering mobility calculated by phase-field simulations was smaller than that predicted using the amount of the excess vacancies induced in the laser-irradiation process, i.e., quenching from the solidus temperature. In the laser-irradiated region, a lot of dislocations were observed by TEM. It is implied that dislocations act as a sink for vacancies and reduce the effect of supersaturated vacancies.

**Keywords:** Additive manufacturing, Powder bed fusion, Antiphase domain, Transmission electron microscope, Computational thermal-fluid dynamics (CtFD) simulation, Phase-Field simulation

# Effect of process parameters on the mechanical properties of maraging steel(18Ni-300) manufactured by powder bed fusion

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## Abstract

Laser Powder Bed Fusion(LPBF) is one of the 3D printing methods that create parts through laser melting. Maraging steel is used in industries such as aerospace, automotive, mold and medical implants, where high-strength parts are required due to its superior strength-to-weight ratio. The process parameters of LPBF include laser power, laser scanning speed, hatch distance, layer thickness, and build direction. These parameters are necessary to produce parts with optimal density and process conditions are required. Otherwise, problems such as porosity and cracks may occur. This study investigates the effect of laser thickness on the mechanical properties of maraging steel. Energy density(J/mm3) conditions for layer thicknesses of 0.04, 0.05 and 0.06um were selected as 50, 71, and 125J/mm3, respectively, laser power and scanning speed were determined accordingly. The study aims to examine the effect of layer thickness process variables of maraging steel manufactured by LPBF process.

**Keywords:** 3D printing, Powder bed fusion, Layer Thickness, Maraging steel, Mechanical properties

| P-E0590 |

# Effects on trace element and carbon on microstructure, mechanical properties and thermal conductivity of the 3D-printed Fe-Cu based alloy using by LPBF process

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## Abstract

With increased interest in metal 3D printing or additive manufacturing (AM) in numerous industries, the need to decrease cost at the alloy level while maintaining mechanical properties must be addressed. Currently, the most common steels used in laser powder bed fusion (LPBF) processes are stainless steels such as 17–4 PH, and 316 L, and hard tool steels such as 18 Ni Maraging 300 and H13. In general, these materials are more costly than most commercial steel grades used in mechanical components and vehicle body structures and have low thermal conductivity. Fe-Cu alloys have received extensive attention due to their excellent mechanical properties, high electrical conductivity and thermal conductivity. In this study, effects of trace element and carbon additions on microstructure, mechanical properties and thermal conductivity of the Fe-Cu based alloy systems manufactured by using LPBF additive process were investigated. These alloys were prepared under an induction melting furnace in a graphite crucible and were manufactured by gas atomization process. The atomized powders were sieved to yield the appropriate particle size range (25–50 μm). L-PBF experiments were carried out with a David 1.0 (merain) machine equipped with a 300W max. In order to examine microstructure, a scanning electron microscope with an energy-dispersive X-ray spectrometer (EDS) and electron backscatter diffraction (EBSD) system. Phase analyses were performed using an X-ray diffractometer with Cu Kα radiation were used. And thermal conductivity was measured at room temperature. Hardness tests were performed using a Vickers test machine

**Keywords:** Fe-Cu alloys, 3D printing, Thermal conductivity, LPBF process

| P-E0597 |

# Effect of Property Differences between Virgin and Used 18Ni300 maraging steel Powders on Mechanical Properties of Additive Manufacturing

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## Abstract

The growth of 3D printing has led to an increasing demand for high-quality powders that can produce reliable and functional parts. Several studies have been published in the past few years that looked at the virgin and used powders and it was observed that morphology, flowability and spreadability can be degraded due to partial sintering and powder recovery. In this study, the differences and properties between virgin and used powders are investigated mainly. This study is conducted in L-PBF 3d printing using maraging steel powders. For particle inspection of virgin and used powders, used X-ray Diffraction, Differential Scanning Calorimeter, Scanning Electron Microscope and X-Ray Fluorescence. The investigation emphasizes the importance of proper powder handling and understanding the powder properties to minimize defects and improve product quality. The presentation concludes that the differences of property of virgin and used powders can induce deterioration of product in 3d printing.

**Keywords:** L-PBF, maraging steel, mechanical properties, selective laser sintering

| P-E0614 |

# Cubic and Epsilon Cobalt Phases in Direct Energy Deposition Additively Manufactured Co-Cr-W Alloy

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## Abstract

Layers of wear-resistant Co-Cr-W alloy are usually hardfaced on stainless steel latch surface of the frequently moving part of nuclear reactor, Control Rod Drive Mechanism (CRDM), and are utilized for the advanced types of nuclear power systems.

In this study StelliteTM 6 alloy powders were deposited on type 304L stainless steel substrate plates by additive manufacturing (AM). More than 90 per cent of the alloy powders were between 53 and 125 micrometer in diameter. AM samples were prepared by direct energy deposition (DED) method with and without preheating of the substrate plate; in other words the substrate plate was hold at 300 degree C or at room temperature to impose two different temperature gradient during the process, respectively. The average deposition layer thickness (or melt pool height) was about 450 micrometer, and ten layers of Co-Cr-W alloy were deposited on each plate.

Cubic and epsilon two cobalt phases were identified by Selected Area Diffraction Pattern (SADP) and Energy Dispersive Spectroscopy (EDS) using Scanning Transmission Electron Microscope (STEM). Orthorhombic M7C3 carbides within the interdendritic region as well as the stacking faults mostly associated with the epsilon phase were also ensured. Wear property of the AM samples were measured by the pin-on-disk tests (ASTM G99-17), and the relevance the test results with the process parameters and consequently with the microstructural features are discussed.

Stellite: Trademark of Kennametal Inc.

**Keywords:** Wear-resistant Cobalt alloy, Control Rod Drive Mechanism (CRDM), Additive Manufacturing (AM), Direct Energy Deposition (DED)

| P-E0649 |

# Study of tensile properties and microstructure according to process parameters of Fe-2.7Mn-6.0Al-0.4C lightweight steel manufactured using DED

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## Abstract

Recently, research on lightweight materials for reducing carbon dioxide emissions is being actively conducted. Among various lightweight materials, Fe-Mn-Al-C lightweight steel is a lightweight steel whose density is lowered by adding Al. High/medium manganese steels have high tensile strength and elongation, but have problems such as difficulty in joining due to large amount of Mn and increase in process cost. In addition, conventional low manganese steels have low tensile strength due to the ferrite and heterogeneous austenite mixture structure. In this study, the goal was to manufacture low manganese lightweight steel by applying the 3D printing process to overcome the low tensile strength of existing low manganese lightweight steel.

Among various 3D printing processes, direct energy deposition (DED) process was used to manufacture low-manganese lightweight steel, we conducted scanning electron microscopy, transmission electron microscopy, electron backscatter diffraction for microstructure analysis. And mechanical properties were analysed through DIC test.

The low-manganese lightweight steel manufactured in this study has secured tensile strength similar to that of existing high/medium-manganese steels, but low elongation compared to high tensile strength remains a challenge.

**Keywords:** Direct energy deposition, Lightweight steel, Low Mn, Laser power

| P-E0659 |

# Microstructure-Based Post-Heat Treatment Design of Inconel 939W fabricated by Laser-Powder Bed Fusion for Creep Enhancement

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## Abstract

Ni-based superalloys are used in gas turbines due to their excellent oxidation resistance and creep characteristics at high temperatures. Various parts with complex cooling channels are being considered to increase turbine efficiency. Conventional casting methods have limitations in complexity, so research on fabricating superalloys using additive manufacturing is underway. While tensile and fatigue properties of additively manufactured parts are equal or superior to cast alloys, creep properties are inferior, and research on appropriate heat treatment is lacking. In this study, we aimed to derive heat treatment to improve the creep properties of additively manufactured Inconel 939W superalloy based on its unique microstructure. When the conventional heat treatment for cast alloys was applied to additively manufactured alloys, creep properties were significantly inferior due to grain boundary liquation, small grain size, and low recrystallization. The solution treatment temperature and time were increased to maximize grain growth and recrystallization. The phase transformation was analyzed through thermodynamic calculations and Differential Scanning Calorimetry to set the highest temperature below the Solidus temperature. The optimal heat treatment induced equiaxed grains with a size of about 200 μm and a recrystallization of over 99%. In addition, the optimal size and distribution of γ' in the γ-matrix were obtained based on the heat treatment variables. Creep test results showed that the proposed heat treatment improved creep life by more than three times compared to conventional heat treatment. The study aims to investigate the microstructural evolution according to heat treatment variables and their impact on creep deformation behavior.

Keywords: Selective laser melting, Inconel 939W, Heat treatment design, Microstructure, Creep

Ni-based superalloys are used in gas turbines and aerospace industries due to their oxidation resistance and creep characteristics at high temperatures. To enhance turbine efficiency, research on superalloy production

Poster Session 1

through additive manufacturing is being conducted for diverse design implementation.

While tensile and fatigue properties in additive manufacturing are comparable or better than cast alloys, creep properties are inferior, with insufficient research on heat treatment. This study aims to derive heat treatment conditions to enhance creep properties based on unique microstructural characteristics of additively manufactured Inconel 939W superalloy.

Applying commercial heat treatment to additively manufactured alloys resulted in lower creep properties due to factors like liquefaction of grain boundaries and low recrystallization rate. To improve this, solution heat treatment temperature and duration were increased to maximize grain growth and recrystallization.

The optimized heat treatment induced equiaxed grains with a size of 180-200 μm and a recrystallization rate above 99%. The study aimed to obtain the optimal size and distribution of γ' according to heat treatment condition variables. The proposed heat treatment conditions improved creep life by more than three times compared to commercial heat treatment. The study examines microstructure evolution based on heat treatment parameters and their influence on creep deformation behavior.

| P-E0697 |

# Understanding the superior mechanical properties of hollow-strut metal lattice materials

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## Abstract

Intricate hollow-strut metal lattice materials are an emerging class of novel metallic cellular materials enabled by additive manufacturing. This work shows that hollow-strut Ti-6Al-4V lattice materials are consistently stronger and stiffer (up to 60% better) than their solid-strut counterparts of the same relative density, both experimentally and through finite element analysis (FEA). The underlying reasons are investigated using analytical models derived from the Timoshenko-beam theory, which considers deformation by concurrent stretching, bending and shear, rather than the single-mode deformation mechanism assumed by the Gibson-Ashby model. Hollow-strut lattices exhibit higher resistance to bending than solid-strut lattices at the same strut length and relative density, thereby leading to increased strength and stiffness. Hollow-strut metal lattices offer an unusual option for lightweight designs, with better mechanical properties at the same or lower density than solid-strut metal lattices.

**Keywords:** Lattice material, Additive manufacturing, Hollow strut, Yield strength, Deformation mechanism

| P-E0868 |

# Ultrastrong yet ductile additively manufactured steel via tailoring austenite stability

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## Abstract

Selective laser melting (SLM) is a very promising near net shape approach to manufacture metallic complex-shaped parts. However, it is highly challenging to manufacture ultrahigh strength medium carbon steels via SLM due to the cracking and low ductility issues. In this contribution, the cracking mechanism of the conventional medium carbon H13 steels during SLM was firstly investigated, which was found to be attributed to the poor stability of retained austenite and the resultant formation of brittle fresh martensite. A modified crack-free H13 steel for SLM was successfully designed via in-situ minor alloying of 316L powders, which substantially enhanced austenite stability. The modified SLM-fabricated H13 steel exhibited an ultrahigh tensile strength of ~2.0 GPa with a total elongation of ~19%. This work demonstrates the critical role of austenite stability in cracking behavior and ductility of the SLM-fabricated medium carbon steels.

**Keywords:** selective laser melting; medium carbon steels; crack; retained austenite; ductility

# POSTER Session 1

## Symposium F : Thin Films and Surface Engineering

**P-F0155** **Comparison of grain growth of poly-Si films deposited with PECVD, LPCVD and sputtering for 3D DRAM application**
Sung Jun Kim (Hanyang University, Korea)

**P-F0157** **Modification of electrical and structural properties at interface between Ru and SiGe with annealing**
Jun Hyeong Park (Hanyang University, Korea)

**P-F0202** **Thermally-induced crystallization of amorphous HfO2 and ZrO2 laminate films**
Kazuma Nagai (Kyushu Institute of Technology, Japan)

**P-F0208** **Distribution and morphology of artificial pinning centers in YBa2Cu3O7-x thin films**
Haruna Nogami (Kyushu Institute of Technology, Japan)

**P-F0248** **Molecular dynamics study of residual stress in diamond-like carbon films during formation process: Impact of substrate material properties**
Noritsugu Kametani (Kyoto Institute of Technology, Japan)

| P-F0155 |

# Comparison of grain growth of poly-Si films deposited with PECVD, LPCVD and sputtering for 3D DRAM application

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## Abstract

Polysilicon(poly-Si) has been widely preferred as a channel material for transistors in semiconductor and display devices due to its moderate mobility and cost-effective fabrication. However, the grain boundary of poly-Si is a dominant leakage path, and it gives worse Ioff than single crystal Si. To reduce the leakage current of poly-Si through its grain boundary, it is considered to secure poly-Si with large and vertically oriented grain to the channel direction. In this work, the grain growth of Si films deposited by using PECVD, LPCVD, and sputtering methods were investigated.

Si films with 25~30 nm thick were deposited on SiO2 with PECVD, LPCVD and sputtering methods, and SiO2 films with 100 nm thick were deposited on Si. Two different samples, one with Si/SiO2 (PO) and the other with SiO2/Si/SiO2 (OPO), were annealed at 700°C, 800°C and 850°C for one hour. The crystallization of Si was measured by spectroscopic ellipsometer (SE), Raman spectroscopy (RS), and TEM.

The SE and RS results showed that the LPCVD and PECVD films had significant increase in crystallinity (from ~9% to ~85%), while the sputtered films had minor increase (from ~38% to ~60%). These tendencies were also observed by TEM, which showed limited grain growth in sputtered sample. Furthermore, TEM image of LPCVD silicon showed vertical grain boundary direction with large grain size compared to other deposition methods. Therefore, LPCVD deposition method could be a suitable deposition method for achieving the desired grain structure for 3D DRAM.

**Keywords:** CVD, sputtering, polysilicon, grain growth, crystallinity

| P-F0157 |

# Modification of electrical and structural properties at interface between Ru and SiGe with annealing

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## Abstract

Ru and SiGe have drawn attention as capacitor electrode and transistor output terminal for next-generation DRAM. Since Ru has less leakage current than TiN, and SiGe has low power consumption and compatibility with existing Si technology. However, in next-generation DRAM with a structure where Ru and SiGe are in direct contact, there is a requirement to form an ohmic contact at the Ru/SiGe interface. In this work, we investigated the modification of properties of the Ru/SiGe interface with annealing temperature.

Ru films was deposited on Si0.2Ge0.8 substrate by ALD, followed by forming gas annealing at various temperature. The electrical properties were measured by 4-point probe. Structural and chemical properties were analyzed with SEM, TEM, XPS and XRD.

It was observed that sheet resistance increased significantly at high annealing temperatures. SEM and TEM analyses showed that Ru and/or Ru compounds were formed in an island-like shape, and SiGe was partially exposed to the surface in 600°C annealed sample. This indicates that rapid increase of sheet resistance at high annealing temperature was caused by agglomeration. XPS analysis showed that Ge diffused towards Ru at 400°C, and both Ge and Si diffused towards Ru at 600°C. It was confirmed that formation of Ru2Ge3 with annealing at 400°C, Ru2Ge3 and Ru2Si3 at 600°C by XRD. In conclusion, we have demonstrated the feasibility of forming Ru germanide through annealing at around 400°C, where agglomeration does not occur. This technique can be applied to the process of reducing contact resistance in Ru/SiGe interface.

**Keywords:** DRAM, Ru/SiGe interface, ohmic contact, agglomeration, forming gas annealing

# Thermally-induced crystallization of amorphous $HfO_2$ and $ZrO_2$ laminate films

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## Abstract

Orthorhombic HfxZr1-xO2 phase is expected to be used as a ferroelectric material. This phase is metastable, and therefore, it is necessary to control its crystal structure to obtain ferroelectricity. Recrystallization of amorphous is a possible way to realize the ferroelectric phase. In this study, we prepared amorphous HfO2 and ZrO2 multilayered thin films and examined their thermally-induced crystalline structures. HfO2 and ZrO2 were alternately deposited on a single crystal Si(100) substrate by radio frequency sputtering. The number of layers was adjusted so that film thickness was 10nm: (0.5 nm+0.5 nm)×10, (1.0nm+1.0nm)×5, (2.5 nm+2.5 nm)×2, (5.0 nm+5.0 nm)×1 layer films. For comparison, solid solution Hf0.5Zr0.5O2 thin film was obtained by co-sputtering HfO2 and ZrO2. The obtained samples were heat treated and examined by grazing incidence x-ray diffraction (GIXRD), x-ray reflectivity (XRR), and transmission electron microscopy (TEM). GIXRD showed that all samples crystallized into the tetragonal and/or orthorhombic phases at 500oC. The layered structure was maintained in (5.0 nm+5.0 nm)×1, (2.5 nm+2.5 nm)×2, and (1.0 nm+1.0 nm)×5 layer films after heat treatment. On the other hand, no layered structure was observed in the as-sputtered (0.5 nm+0.5 nm)×10 layer film. After crystallization, it was confirmed that (5.0 nm+5.0 nm)×1-layer film had the same crystallographic orientation between HfO2 and ZrO2 layers. Nano-beam electron diffraction patterns of these samples were found to be orthorhombic (space group: Pca21), confirming the existence of orthorhombic crystalline phase.

**Keywords:** HfO2, ZrO2, ferroelectric, amorphous, crystallization

# Distribution and morphology of artificial pinning centers in $YBa_2Cu_3O_{7-x}$ thin films

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## Abstract

The critical current density of the superconductor YBa2Cu3O7-x(YBCO) can be effectively improved by doping artificial pinning centers (APCs) that fix the quantized magnetic flux through the superconductor. For superconducting wire applications, it is of technological importance for introducing APCs uniformly over a large scale. Few studies have paid attention to the distribution and structure of APCs throughout YBCO thin films. In this study, YBCO thin films doped with high concentration APCs were prepared to examine their distribution and morphology. The thin films were deposited on SrTiO3 (STO) or LaAlO3 (LAO) substrates using pulsed-laser deposition. YBCO + 8.0 vol.% BaSnO3 (BSO) and YBCO + 15.0 vol.% Ba2LuNbO6 (BLNO) were used as targets. The substrate temperature and laser frequency during deposition were 890 °C and 2 Hz, respectively. The as-deposited specimens were fabricated into cross-sectional and plan-view samples using focused ion beam, and characterized by scanning electron microscopy, transmission electron microscopy, and energy dispersive X-ray spectroscopy. It was confirmed that the APCs with different morphologies are heterogeneously distributed in the YBCO matrix: regions with precipitates and nanorods exist as well as regions with almost no precipitates. As a characteristic structure of the BLNO-doped sample, the precipitation of the nanorod material was observed along substrates, suggesting high crystallinity despite the high concentration of BLNO in the sample. Also, the BLNO nanorods were segmented by YBCO layers which was presumably introduced to release strain.

**Keywords:** artificial pinning centers, YBa2Cu3O7-x, TEM, superconductor, pulsed-laser deposition

| P-F0248 |

# Molecular dynamics study of residual stress in diamond-like carbon films during formation process: Impact of substrate material properties

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## Abstract

Diamond-like carbon (DLC) films have superior tribological properties and can be applied to a variety of base materials. However, DLC films are prone to delamination due to high residual stress, limiting their application to substrates with low thermal conductivity that are difficult to deform. In addition, because DLC films are amorphous, stress measurement by X-ray diffraction is not possible. Therefore, the local stress state of the films must be predicted through simulation.

Recently, we performed molecular dynamics simulations to evaluate the effects of sp2 hybridization (graphite structure) and sp3 hybridization (diamond structure) in DLC films deposited on carbon diamond substrates on the residual stresses in the films [N. Kametani et al., Comput. Mater. Sci., 209 (2022) 111420]. We found that the origin of the compressive residual stress in the films is the structural change from sp2 to sp3 during the deposition process.

In this study, molecular dynamics simulations of DLC film formation were performed to investigate the effects of substrate materials on the residual stress generated in films and the formation of carbon bonds during film formation. The results showed that sp3 clusters in the films grow to a larger size on Fe substrate than on diamond substrate. This causes higher compressive residual stresses in the Fe substrate. These phenomena were discussed in detail in terms of energy during film growth and differences in substrate thermal conductivity.

**Keywords:** Diamond-like Carbon, Deposition Process, Residual Stress, Mechanical Property, Molecular Dynamics

# POSTER Session 1

## Symposium G : Materials for Energy Storage and Generation

**P-G0025** **Development of Technology for Manufacturing Simulated Test Rods and Shields Using High-performance Neutron Absorbing Materials**
Seung Youb Han (Korea Atomic Energy Research Institute, Korea)

**P-G0028** **Effect of ash content on charge-discharge properties of needle coke based artificial graphite**
Yuan Gao (Ansteel Beijing Research Institute Co.LTD, China)

**P-G0045** **High-Energy Long-life Lithium-Sulfur Batteries via Redox-Active Interlayer Strategy**
Jong-Sung Yu (Daegu Gyeongbuk Institute of Science & Technology (DGIS), Korea)

**P-G0065** **Bimetallic Ni-Fe-S nanoparticles directly grown on porous MXene substrate as bifunctional electrocatalyst for water electrolysis**
Kyeongseok Min (Inha University, Korea)

**P-G0068** **Self-templating construction of Fe, F dual-doped CoS2 hollow nanospheres for highly efficient oxygen evolution reaction**
Hyejin Kim (Inha University, Korea)

**P-G0076** **Co, N co-doped Ni2P on Ni foam as a bifunctional electrocatalyst for oxygen evolution reaction and urea oxidation reaction**
HAE MIN SEONG (Inha University, Korea)

**P-G0096** **Interface engineering strategy to optimize the electronic structure of CoFe LDH via hybridization with oxygen vacancy-enrich Co3O4 for efficient oxygen evolution reaction**
Junseong Kim (Inha University, Korea)

**P-G0121** **Highly Breathable, Water-Resistant, and Self-Healing Fibrous Triboelectric Nanogenerators for Enhanced Performance in Wearable Electronics**
Duc Khanh Tran (Sungkyunkwan University, Korea)

**P-G0424** **Radiation induced hardening of Fe-Mn-Ni alloys under irradiation**
Hideo Watanabe (Kyushu University, Japan)

# POSTER Session 1

P-G0473 **Improvement of electrical power generation from lead zirconate titanate piezoelectric ceramics**
Itsuki Shimazu (Okayama University, Japan)

P-G0537 **The Role of Transition Metal Doping in Enhancing Hydrogen Storage Capacity in Porous Carbon Materials**
Xue Gao (South China University of Technology, China)

P-G0545 **Effect of Rhenium Addition on Microstructure and Mechanical Properties of Ni-16Mo ODS Alloys for Next Generation Energy Applications**
Sanghoon Noh (Pukyong National University, Korea)

| P-G0025 |

# Development of Technology for Manufacturing Simulated Test Rods and Shields Using High-performance Neutron Absorbing Materials

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## Abstract

A marine reactor is performed a boric acid-free operation for long-term operation, reduction of reactor volume, and simplification of a system structure. Therefore, it is necessary to control the core power distribution and excess reactivity with only the burnable poison and the control rod. For the reasons mentioned above, neutron absorbers with various neutron absorption capacities are required depending on the location of the core, and the absorber must maintain structural integrity according to irradiation and thermal changes during the period of use. In order to vary the neutron absorbing ability, high and low concentration neutron absorbers manufacture to adjust the concentration of the neutron absorbing material in the rod. The performance requirements of neutron absorbers suitable for marine reactors were considered, and basic physical properties were studied by selecting Gd2O3-Y2O3 and Dy2O3-Y2O3 oxides as suitable absorber candidates. The manufacturing process of the prototype sintered body with two compositions was developed, and the thermal properties of the prototype sintered body were evaluated. In order to evaluate the irradiation characteristics of the high-performance neutron absorber, test rods loaded with Gd2O3-Y2O3 and Dy2O3-Y2O3 neutron absorbers were prepared, respectively. Shield manufacturing technology was developed using the developed neutron absorbing material. The material design of the shield was carried out by selecting a material to shield the gamma rays with absorb the neutron. In addition, the applicability of the 3D printing additive manufacturing process was evaluated so that it can be applied to the production of complex structures and the repair of existing products.

**Keywords:** Marine reactor, Neutron Absorbing Materials, Simulated Test Rod, Neutron Shield

| P-G0028 |

# Effect of ash content on charge-discharge properties of needle coke based artificial graphite

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## Abstract

With the development of lithium ion battery industry and technology, artificial graphite, as the most widely used negative electrode material of lithium ion battery, has the advantages of low cost, good recycling performance and wide range of raw materials. The main raw materials of artificial graphite include oil-based needle coke and coal-based needle coke. Coal based needle coke mainly made through delayed coking technology using coal tar pitch as raw material. Compared with the catalytic cracking slurry used in oil based needle coke, the ash content of coal tar pitch is higher. It is generally believed that the ash content of needle coke will be retained in artificial graphite products, which will have a negative impact on the performance of lithium ion intercalation, but there is no clear conclusion on the level of ash content and the specific extent of its impact. At present, in this study, the author uses needle coke with different ash content as raw material, adopts the same grinding, grinding, granulation and graphitization process to make artificial graphite anode material, and the two materials are assembled into lithium ion battery for charging and discharging test, the results show that the coal-based artificial graphite has the first discharge specific capacity close to the theoretical value. The discharge specific capacity of 360mAh/g is still maintained after 30 cycles, while the discharge specific capacity of oil based needle coke is 340mAh/g, so coal based needle coke may be an ideal raw material for high capacity anode materials.

**Keywords:** needle coke, artificial graphite, ash content, lithium ion battery, anode material.

| P-G0045 |

# High-Energy Long-life Lithium-Sulfur Batteries via Redox-Active Interlayer Strategy

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Lithium-sulfur batteries have theoretical specific energy higher than state-of-the-art lithium-ion batteries. However, from a practical perspective, these batteries exhibit poor cycle life and low energy content owing to the polysulfides shuttling during cycling. To tackle these issues, researchers proposed the use of redox-inactive protective layers between the sulfur-containing cathode and lithium metal anode. However, these interlayers provide additional weight to the cell, thus, decreasing the practical specific energy. Here, we report the development and testing of redox-active interlayers consisting of sulfur-impregnated polar ordered mesoporous silica. In this case, interestingly, sulfur storage/trapping occur at the polar silica while electron transfer at conducting agent in the interlayer comprising sulfur-loaded platelet ordered mesoporous silica (pOMS/Sx IL) during charge-discharge. Differently from redox-inactive interlayers, these redox-active interlayers enable the electrochemical reactivation of the soluble polysulfides, protect the lithium metal electrode from detrimental reactions via silica-polysulfide polar-polar interactions and increase the cell capacity. Indeed, when tested in a non-aqueous Li-S coin cell configuration, the use of the interlayer enables an initial discharge capacity of about 8.5 mAh cm-2 (for a total sulfur mass loading of 10 mg cm-2) and a discharge capacity retention of about 64 % after 700 cycles at 335 mA g-1 and 25 °C.

**Keywords:** Li-S battery, redox-active system, interlayer, platelet ordered mesoporous silica host, polar-polar interaction

| P-G0065 |

# Bimetallic Ni-Fe-S nanoparticles directly grown on porous MXene substrate as bifunctional electrocatalyst for water electrolysis

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## Abstract

Among the various renewable energy sources, hydrogen (H2) is considered as most promising substance in future energy society owing to its high energy density and environmental friendliness. Recently, electrochemical water splitting, which is consisted of anodic oxygen evolution reaction (OER) and cathodic hydrogen evolution reaction (HER), has great potential for high-purity hydrogen production. However, the practical efficiency of water electrolysis is limited due to the intrinsically sluggish reaction kinetics of OER and HER. To date, the precious metal-based electrocatalysts such as RuO2 and Pt/C were employed as state-of-the-art electrocatalysts forwater electrolysis. However, due to the high expense, mono-functionality, and unsatisfactory stability of them, research on bifunctional electrocatalysts with low cost and high activity has become an urgent topic.

In this work, 2D-structured titanium carbide (Ti3C2) MXene was employed as an efficient substrate for growth of active species with plentiful terminal groups (-OH, -O, -F). The MXene has outstanding hydrophilicity and electrical conductivity, leading to the enhanced electrocatalytic activity in aqueous alkaline solution. To improve electrochemical surface area and introduce channels for mass transport, we generated abundant pore in 2D-structured Ti3C2 substrate. Additionally, the insufficient redox property of the Ti3C2 was improved via direct growth of Ni-Fe-S with atomic ratio of Ni:Fe=3:1 using one-step solvothermal process. As a result, the prepared electrocatalyst exhibited excellent electrocatalytic activity with low overpotential of 309 and 148 mV at 10 mA cm−1 for OER and HER, respectively. Additionally, the Ni-Fe-S/porous-MXene showed exceptional stability during the continuous water electrolysis for 100 h.

**Keywords:** electrocatalyst; oxygen evolution reaction; hydrogen evolution reaction; MXene; bimetal sulfide

| P-G0068 |

# Self-templating construction of Fe, F dual-doped CoS2 hollow nanospheres for highly efficient oxygen evolution reaction

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## Abstract

Due to the serious energy crisis and environmental problems, developing clean and highly efficient energy sources has been received extensive attention. Electrochemical water splitting, which can produce ultrapure hydrogen gases, is consisted of anodic oxygen evolution reaction and cathodic hydrogen evolution reaction. Notably, the complicated reaction mechanism of OER with four-electron transfer process causes significant overpotential, thereby resulting in poor electrochemical efficiency for overall water electrolysis. Until now, noble metal-based oxide materials (IrO2 and RuO2) were employed as state-of-the-art electrocatalyst owing to the superior OER activity. However, their high cost and unsatisfactory long-term durability hinder the large-scale application of water electrolysis. Therefore, a lot of researchers have devoted to developing non-noble metal-based electrocatalysts with low cost, enhanced OER activity, and electrochemical durability.

Herein, we proposed facile and readily scalable synthetic method of hollow-structured Fe, F dual-doped CoS2 nanosphere (Fe-CoS2-F) using Co-glycerate nanosphere as a self-sacrificial template. The Co-glycerate solid sphere was converted into hollow-structured bimetallic CoFe-PBA via simple anion exchange process at room temperature. Subsequently, simultaneous sulfidation and fluorination process was conducted by heat treatment under Ar atmosphere, thereby resulting in hollow-structured Fe-CoS2-F. As a result, the Fe-CoS2-F electrocatalyst exhibited remarkable electrocatalytic performance toward OER with small overpotential (298 mV at a current density of 10 mA cm−2), low Tafel slope (46 mV dec−1), and robust long-term durability (over 100 h) in alkaline electrolyte. Therefore, this study would provide new insight into the development of noble metal-free materials for diverse energy storage and conversion applications.

**Keywords:** oxygen evolution reaction; transition metal; electrocatalyst; dual-doping; hollow structure

| P-G0076 |

# Co, N co-doped $Ni_2P$ on Ni foam as a bifunctional electrocatalyst for oxygen evolution reaction and urea oxidation reaction

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## Abstract

Water electrolysis is considered as promising technology for high-purity hydrogen production without emission of environmental pollutants. However, the sluggish kinetics of anodic oxidation reaction (OER) induce the low coulombic efficiency of overall water electrolysis. To address this issue, the OER could be replaced by thermodynamically favorable urea oxidation reaction (UOR). Furthermore, abundant urea species in wastewater can be effectively purified via the electrocatalytic UOR process. To date, the expensive noble metal-based materials have been employed as state-of-the-art electrocatalyst for water oxidation. Therefore, many researchers have devoted to developing UOR electrocatalysts with low cost and high electrocatalytic activity to conduct hydrogen production and wastewater purification, simultaneously.

In this study, we prepared Co, N dual-doped Ni2P (Co-Ni2P-N) directly grown on Ni foam (NF) as a bifunctional electrocatalyst for OER and UOR. The as-synthesized Co-Ni2P- N/NF electrocatalyst exhibited the excellent electrocatalytic performance toward OER with the overpotential of 329 mV to deliver 100 mA cm−2 and the remarkable stability during 100 h. For UOR, the low potential of 1.39 V vs. RHE was required at 100 mA cm−2, and electrocatalytic performance was retained over 100 h. The enhanced electrocatalytic performance of Co-Ni2P- N/NF is mainly attributed to the moderately adjusted surface electronic structure via simultaneous introduction of Co, N dual dopants into Ni2P structure. This research would provide the new insight into the development of efficient electrocatalyst for energy conversion and storage system and wastewater treatment.

**Keywords:** electrocatalyst; dual doping; phosphidation; oxygen evolution reaction; urea oxidation reaction

| P-G0096 |

# Interface engineering strategy to optimize the electronic structure of CoFe LDH via hybridization with oxygen vacancy-enrich $Co_3O_4$ for efficient oxygen evolution reaction

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## Abstract

The development of clean and sustainable energy has attracted significant attention due to increasing concerns about global warming and the depletion of fossil fuels. Electrochemical water splitting is considered a promising strategy due to its eco-friendliness and high-purity H2 production. However, the large overpotentials caused by sluggish four-electron reaction during the anodic oxygen evolution reaction limited their large-scale application. Until now, the precious metal-based OER catalysts, such as Ir/Ru based oxide, have been used as state-of-art OER electrocatalyst. Nevertheless, their high cost, scarcity, and low stability have seriously hindered large scale commercialization. Therefore, numerous researchers have been studied about transition metal-based catalysts owing to their low cost, earth-abundance and excellent long-term stability.

In this study, we synthesized oxygen defect-rich Co3O4/CoFe-LDH composite on carbon matrix (CoFe-LDH/Vo-Co3O4@C) via co-precipitation, annealing process, and subsequent sonochemistry method. Spinel-structured cobalt oxide is an efficient electrocatalyst due to its high corrosion resistance and rich redox properties. Oxygen defect on the surface of Co3O4 can improve electrical conductivity and modulate the adsorption/dissociation energy states. Furthermore, interfacial junction of Co3O4 with CoFe LDH, which is well known as OER catalyst, can effectively enhance the intimate interaction with oxygen containing intermediates. As expected, the obtained CoFe-LDH/Vo-Co3O4@C showed outstanding OER performance with an overpotential of 298 mV at 10 mA cm-2 and Tafel slope of 60.2 dec-1. In addition, the prepared electrocatalyst exhibited excellent long-term stability for 30 h. This research will provide new insights for preparation of transition metal-based composite materials for future energy storage and conversion system.

**Keywords:** oxygen evolution reaction, layered double hydroxide, oxygen vacancy, electrocatalysts

| P-G0121 |

# Highly Breathable, Water-Resistant, and Self-Healing Fibrous Triboelectric Nanogenerators for Enhanced Performance in Wearable Electronics

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## Abstract

The potential of triboelectric nanogenerators (TENGs) to harvest electricity from mechanical movements has been widely recognized, paving the way for innovative energy harvesting solutions in various applications. While numerous studies have focused on thin-film-based TENGs due to their ability to generate appreciable voltage and current levels, these devices pose challenges in wearable applications as their rigid structure inhibits sweat evaporation. In contrast, fibrous TENGs offer superior breathability but are vulnerable to performance degradation caused by external factors such as high humidity or continuous working cycles. In this study, we develop a novel triboelectric nanogenerator that combines the advantages of both structures while overcoming their limitations through the use of water-resistant materials to improve durability and performance. Our TENG design employs polybutadiene-based urethane (PBU) and polyvinylidene fluoride (PVDF) as charge donor and acceptor materials, respectively. These materials contribute to the TENG's water-resistant nature, ensuring consistent performance under varying environmental conditions. Electron transfer to the external circuit is facilitated by Ni-Cu conductive textiles, further enhancing the TENG's overall performance. One of the key features of the proposed TENG is its self-healing capability, enabled through a simple solvent vapor method. This allows the device to recover its initial performance following damage or wear, extending its operational lifespan. Under low stress and frequency conditions, our TENG was able to generate approximately 120 Volts and an alternating current of 10 μA. Remarkably, these performance parameters were maintained even after thousands of vertical contact-separation cycles, demonstrating the TENG's durability and resilience. To showcase the practical applications of our fibrous TENG, we successfully illuminated a series of LEDs and an Alternating Current Electroluminescence (ACEL) device using the harvested energy. This highlights the potential for the TENG's integration into self-powered wearable electronics. Our research introduces a groundbreaking approach to the design and development of wearable electronics that boast long-lasting performance, easy washability, and uncomplicated self-healing capabilities. The breathable, water-resistant, and self-healing fibrous TENG offers promising prospects for advancing wearable technologies and energy harvesting solutions across various industries.

**Keywords:** Triboelectric nanogenerators, Self-healable polymers, Wearable electronics, Fibers

Poster Session 1

| P-G0424 |

# Radiation induced hardening of Fe-Mn-Ni model alloys under Irradiation

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## Abstract

The neutron irradiation of Fe based model alloys and steels leads to an increase in the ductile-to-brittle transition temperature (DBTT) with a decrease in the upper shelf energy. It is well known that the Cu content has a strong influence on the embrittlement phenomena; especially, the Cu-rich precipitates have been thought to be directly responsible for the embrittlement. In contrast, mechanical property studies for the steels with different Cu levels have shown that so-called matrix defects are dominant in the embrittlement of low-Cu steels as well as in that of high-Cu steels at high fluences. To study the effect of dislocation loop formation at high fluencies and high flux on radiation hardening in those steels, neutron and ion irradiation have been conducted for Fe-based model alloys with different Ni and Mn levels. The neutron irradiation was performed in BR2 (BAMI and CALLIST) . Hardness tests were conducted before and after the irradiation at room temperature. After the irradiations, microstructure was observed by Cs–corrected microscope (ARM200FC).

The hardness increases with irradiation dose. STEM-EDS observation revealed that this is due to the formation of very high density of interstitial type dislocation loops at lower temperature. On the other hand, at 563K, small loops and solute clusters of about 2nm were formed in matrix and also in the vicinity of dislocation. The recovery behaviour of the hardness by post-irradiation annealing at 723K was related with disappearance of these loops.

**Keywords:** Radiation induced hardness, defect clusters, STEM-EDS, Neutron irradiation

| P-G0473 |

# Improvement of electrical power generation from lead zirconate titanate piezoelectric ceramics

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## Abstract

Lead zirconate titanate (PZT) piezoelectric ceramics have unique material properties, such as the piezoelectric and inverse piezoelectric effects. With the effects, PZT ceramics have been employed for various engineering components, e.g., sensors, buzzers and actuators. In recent years, due to environmental issues, the piezoelectric ceramics have been used for clean energy system. One of the systems is designed with setting the PZT ceramic plates on the ground, i.e., floor power system, in which mechanical energy applies to the PZT ceramics with the steps taken by a person walking. Some of the related systems have been temporarily tested at ticket gate of station hall. However, this system has received insufficient electric power generation due to the low energy efficiency. To solve the issue, an attempt was made to improve the energy efficiency via various loading conditions. Two main approaches were conducted in the present work: (i) different fixing conditions and (ii) different stress fields of the PZT ceramic plate. The aim of the former approach is to obtain high resonance frequency from both PZT ceramics and the experimental setup. Electric power generation was influenced particularly by the relationship between the stiffness of the PZT ceramic and loading frequency. The later experiment was conducted to increase electric power generation via different internal stain of PZT ceramics under various stress fields. Stress fields affected the efficiency of electric power generation: the high compressive stress to the PZT ceramics with direction perpendicular to the c-axis of tetragonal structure leads to high electric power generation.

**Keywords:** PZT, Piezoelectric effects, Electric power generation, Fixing condition, Stress field

| P-G0537 |

# The Role of Transition Metal Doping in Enhancing Hydrogen Storage Capacity in Porous Carbon Materials

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## Abstract

Porous carbon materials hold great promise for hydrogen storage applications due to their remarkable characteristics, including light mass, high theoretical H2 storage capacity, and fast kinetics. However, the weak van der Waals forces between carbon materials and H2 limit its application. To address this issue, surface modifications such as incorporation metal active sites, heteroatomic doping, and introduction defects can enhance the interaction between H2 and materials. In this study, porous carbon materials (PCMs) doping with transition metal single atoms (PCM-TMs, TM: Mn, Fe, Ni) were prepared to investigate the role of TM doping. The developed PCM-TMs exhibited a high specific surface area (up to 1363 m2/g) and pore volume (up to cm3/g). Experimental results revealed that PCM-TMs displayed significantly improved H2 storage capacity, usable capacity, and H2 uptake per specific surface area (SSA) compared to PCM. Moreover, PCM-TMs exhibited a higher isosteric heat of adsorption (Qst) than PCM, indicating enhanced interaction between H2 and carbon materials. Theoretical calculations demonstrated that this interaction involved a nearly weak chemisorption force (~9.27 kJ/mol). Remarkably, Mn-doped porous carbon material

(PCM-Mn) exhibits a hydrogen storage capacity of ~3.45 wt.% (20.44 g/L) at 77 K (35 bar-H2). Even at 253 K (50 bar-H2), the capacity can reach ~1.41 wt.% (8.34 g/L). The H2 uptake per SSA for PCM-Mn reaches 1.03×10-3 wt.% / g·cm-2 (253 K, 50 bar-H2), which is 1.5 times larger than that of PCM. This study provides valuable insights into enhancing the H2 storage performance of porous carbon materials.

**Keywords:** hydrogen storage, porous carbon materials, transition metals, physisorption, isosteric heat

| P-G0545 |

# Effect of Rhenium Addition on Microstructure and Mechanical Properties of Ni-16Mo ODS Alloys for Next Generation Energy Applications

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## Abstract

Oxide Dispersion Strengthened (ODS) alloy is one of the heat-resistant alloys which have thermo-chemically stable nano-sized oxide particles in a metal matrix. Recently, this alloy is considered to be mainly used as structural materials for marine, aerospace, thermal power and nuclear/fusion systems. To improve the mechanical properties at elevated temperatures, some strengthening mechanisms such as solid-solution hardening and precipitation hardening are applied by additions of various alloy elements. In particular, it is well known that Rhenium effectively inhibits the coarsening of the γ' phase due to extremely low diffusion coefficient in nickel-based alloys. This suppression of γ' coarsening is recognized to enhance creep and fatigue properties at elevated temperatures. Al is one of the solid-solution hardening elements, which also improves oxidation resistance by a forming of passive films on the surface. In this study, the rhenium effect on the microstructure and mechanical properties of Ni-16Mo ODS alloy were investigated. Alloy specimens with Ni(bal.)-16Mo-4.5Al in wt. % were fabricated by mechanical alloying and hot isostatic pressing processed to evaluate the tensile properties at room and elevated temperatures. Microstructural changes according to the rhenium contents were observed by electron microscopes. It was possible to confirm the effect of Re additions in Ni-based ODS alloy, and is expected to develop the new structural materials for the next generation energy applications.

**Keywords:** Ni-based ODS alloy, Rhenium, Microstructure, tensile properties, solid-solution hardening

# POSTER Session 1

## Symposium H : Electronic and Magnetic Materials

**P-H0365** **Enhancement of Hard Magnetic Properties by Substitution on Fe2+ sites of W-type Hexaferrites**
Min-Kyung Seong (Sookmyung Women's University, Korea)

**P-H0366** **Cooling Rate Influence on Microstructure and Magnetic Properties in FeCo-2V Electrical Steels**
Jihye Park (Sookmyung Women's University, Korea)

**P-H0388** **Study on Structural Characteristics and Magnetic Properties of Ultra-thin Pure Iron Ribbons with Various Annealing Temperatures**
Xiaotong Ma (Tohoku University, Japan)

**P-H0570** **Phase selection in Mn-Bi-Sb ternary system by in-magnetic-field annealing**
Ryota Kobayashi (Kagoshima University, Japan)

**P-H0575** **First-principles study of surface anomalous Hall effect in van der Waals antiferromagnets**
Yume Morishima (Kanazawa University, Japan)

**P-H0622** **Effects of Fine Nb Addition and Heat Treatment on Soft Magnetic Properties**
Hyunkyung Lee (Sookmyung Women's University, Korea)

**P-H0647** **Reinforcement of Soft Magnetic Properties by Heat Treatment in Melt-spun Fe-based Ribbons**
Jiyoon Lim (Sookmyung Women's University, Korea)

**P-H0959** **Tailoring the magnetic properties of Sm-Co nanocomposites through morphological evolution via HCl washing**
Kavita Kumari (Changwon National University, Korea)

**P-H0987** **Approach to improve the MHz performance of Fe-Si based soft magnetic composites**
Xiaowei Jin (Lanzhou University, China)

**P-H1181** **Characterization of Fe-6.5% Si steel sheet produced 3D Printing**
Semin Park (Pukyung National University, Korea)

**P-H1183** **Study on Moisture Trigger Self-Healing Effect of Ti3C2Tx MXene Electrode with Application**
Jun Sang Choi (Sungkyunkwan University, Korea)

| P-H0365 |

# Enhancement of Hard Magnetic Properties by Substitution on $Fe^{2+}$ sites of W-type Hexaferrites

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## Abstract

W-type hexaferrite is a type of hexaferrite with high saturation magnetization (Ms) of 78-80 emu/g, anisotropy field (Ha) of 19 kOe, and ferromagnetic resonance (FMR) frequencies of 30-60 GHz. These features make it a versatile material with a unique crystal structure and magnetic properties that make it suitable for various applications, including electromagnetic wave absorbers and nonconductive permanent magnets. However, despite its potential with large saturation magnetization (Ms), the study of the hard magnetic properties of W-type hexaferrite is less due to its relatively low coercivity (Hc) than M-type hexaferrites. This paper aims to enhance the hard magnetic properties of the W-type hexaferrite, particularly its coercivity (Hc), without decreasing saturation magnetization (Ms). This study used a conventional ceramic process (solid-state reaction) to synthesize the W-type hexaferrites in the air. The W-type hexaferrite structure contains Fe2+ and Fe3+, with Fe2+ being unstable at low temperatures and atmospheric pressure. To stabilize the W-type hexagonal structure, the Fe2+ was replaced with Zn2+ and Ni2+. We substituted Ni2+, Zn2+ and additional element on Fe2+ side to enhance higher coercivity while remaining saturation magnetization over 70 emu/g. The substitution effects on the structure and magnetic properties were investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), and vibrating sample magnetometry (VSM).

**Keywords:** W-type hexaferrite, permanent magnet, coercivity, solid-state reaction

| P-H0366 |

# Cooling Rate Influence on Microstructure and Magnetic Properties in FeCo-2V Electrical Steels

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## Abstract

As the market size of electric vehicles increases and competition between companies intensifies, the demand for materials for high-performance traction motors is increasing. Electrical steel for high-performance motors is a soft magnetic material with high saturation magnetic flux density and low iron loss. Among materials known so far, a promising candidate that satisfies high saturation flux density and low core loss is FeCoV alloy. The FeCo binary alloy is a soft magnetic material with a saturation magnetic flux density of 2.4 T, low iron loss, and coercive force. Adding 2 to 4% of vanadium reduces the brittleness of the alloy and improves workability during the rolling process without deteriorating magnetic properties. Therefore, FeCoV alloys will likely be used in fast-growing electric vehicles and high-efficiency motors required in the future EV market. In addition to the strength of this alloy, if the motor runs under a low applied magnetic field, it can run at a low current, which in turn gives an energy-saving effect. In order to have a high saturation magnetic flux density even in a low applied magnetic field, the magnetic permeability must be maximized; thereby, adjusting the initial magnetization curve becomes an important variable. In addition, it was confirmed that the internal microstructure and residual stress were affected by the final annealing conditions. The degree of vacuum in the furnace and annealing temperature/time greatly affect soft magnetic properties such as saturation magnetic flux density and energy loss. For this reason, in this study, the effect of magnetic and structural characteristics according to heat treatment conditions was investigated for application to a high-performance traction motor, and the permeability was maximized by raising the initial magnetization curve.

**Keywords:** FeCoV alloy, soft magnetic properties, electrical steels, annealing, cooling rate

| P-H0388 |

# Study on Structural Characteristics and Magnetic Properties of Ultra-thin Pure Iron Ribbons with Various Annealing Temperatures

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## Abstract

Soft magnetic ribbons with the thickness more than 20 μm are typically used for the application such as transformers, inductors and so on because of their high magnetic flux density and low hysteresis losses. As for the ribbons with the thickness less than 20 μm, their fundamental properties are not well explored. Herein, we focused on ultra-thin pure Fe ribbons with high magnetic flux density, investigated the structural characteristics and magnetic properties of these ribbons with and without annealing and further discussed the influence of annealing temperatures (Ta) on their properties in detail.

The crystal orientation changes from (200) and (211) to random one for Ta > 1173 K, which might be attributed to both the internal stress and recrystallization. In contrast, the permeability value increases as Ta increases up to 1173 K, reaches maximum at Ta = 1173 K, and further decreases for Ta > 1173 K. This behaviour may be originated from the change in structural characteristics of the Fe ribbon with Ta. These results means that structural characteristics and magnetic properties of ultra-thin pure Fe ribbons are markedly influenced on the annealing temperature.

Acknowledgment

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**Keywords:** Magnetic losses, Power electronics, Soft magnetic materials, Transformer cores.

| P-H0570 |

# Phase selection in Mn-Bi-Sb ternary system by in-magnetic-field annealing

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Ferromagnetic phases are stabilized in a magnetic field by the gain of Zeeman energy. Therefore, phase equilibrium and phase transformations can be controlled by magnetic fields [1]. In Mn-Bi binary system, the synthesis of ferromagnetic MnBi from nonmagnetic Mn and Bi is enhanced by in-magnetic-field annealing [2]. Mn-Bi and Mn-Sb binary system have various magnetic phases such as ferromagnetic MnBi, ferromagnetic Mn1.1Sb, and ferrimagnetic Mn2Sb. In this study, in-magnetic-field annealing of Mn-Bi-Sb ternary system was carried out.

Mn, Sb, and Bi powder with molar ratio of 2:1:1 was reacted at 523 and 573 K in magnetic field up to 15 T. The reacted phases were evaluated by X-ray diffraction measurements (XRD). Magnetization was evaluated by vibrating sample magnetometer at room temperature.

The obtained phase at 523 K at 0 T was small fraction of Mn1.1Sb phase in addition to Bi-Sb eutectic phase, and Mn. The phase fraction of Mn1.1Sb became larger at 15 T. On the other hands, Mn2Sb + Bi was stable at 573 K. The reacted phase was not influenced by magnetic field. On the other hand, ferromagnetic MnBi phase was not observed for all conditions. Therefore, it was found that Mn+ Bi-Sb phase, Mn1.1Sb + Mn + Bi-Sb phase, and Mn2Sb + Bi were selectively synthesized by combination of annealing temperature and magnetic field intensity.

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**Keywords:** Magnetic field, Reaction, Magnetic materials

| P-H0575 |

# First-principles study of surface anomalous Hall effect in van der Waals antiferromagnets

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## Abstract

The thermoelectric effect, which produces an electric field from a temperature gradient, has potential applications in terms of energy conservation. The anomalous Nernst effect (ANE) in magnetic materials is a transverse thermoelectric effect that generates an electric field in the direction of the cross-product of the temperature gradient and the magnetization or virtual magnetic field of materials. Due to the simplicity of thermoelectric conversion modules, ANE has recently attracted the attention [1]. ANE requires the generation of anomalous Hall effect (AHE), and it has been believed that AHE cannot occur without magnetization. Recently, however, AHE and ANE in antiferromagnets have been reported, following the report of AHE in Mn3Sn, a chiral antiferromagnet [2].

MnBi2Te4 was found as a magnetic topological insulator with interlayer antiferromagnetic ordering [3] and predicted to be antiferromagnetic axion insulators in even layers [4] and ferrimagnetic Chern insulators with large anomalous Nernst coefficients (ANCs) in odd layers [4,5]. MnBi2Te4 with an antiferromagnetic axion insulator phase is expected to cause surface AHE with different signs of surface anomalous Hall conductivities (AHCs) at the upper and lower surfaces [6], while the entire system does not induce AHE. In our study, we calculated layer-decomposed AHCs in MnBi2Te4 with even layers and considered ANE arising from the surface AHE to expand the possibilities of ANE with antiferromagnets. In the presentation, we will report the layer-decomposed AHCs, ANCs, and thermoelectric figure of merits in MnBi2Te4 with even layers and another antiferromagnetic van der Waals layer materials.

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**Keywords:** anomalous Hall effect, anomalous Nernst effect, van der Waals material, antiferromagnetism, first-principles calculation

# Effects of Fine Nb Addition and Heat Treatment on Soft Magnetic Properties

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## Abstract

This study investigated the effects of adding Nb to a Fe-based alloy, aiming to enhance its properties for these applications. Induction and arc melting techniques were employed in an argon atmosphere, using high-purity metals, to ensure uniformity. The resulting ribbon samples, obtained through melt spinning, measured 2-3 mm in width and 20-30 μm in thickness. Various properties of these ribbons were analyzed to assess their suitability for the intended applications. The thermal properties of the alloy were evaluated using a DSC. It was observed that the addition of Nb led to improved thermal stability. As the Nb content increased, the first crystallization temperature reached its maximum at 701 K. XRD analysis confirmed that the structural characteristics of the ribbon samples remained amorphous. Magnetic properties were examined using a VSM. Including Nb resulted in a decrease in coercivity, indicating the development of soft magnetic properties. However, the saturation magnetization decreased with higher Nb content. To address this, annealing was performed. The annealing conditions were determined according to the DSC results of the as-spun ribbon, with annealing temperatures ranging from 20 K intervals. XRD analysis of the annealed ribbon samples confirmed the presence of the α-Fe phase. The VSM results showed that the saturation magnetization reached its highest value at 214.97 emu/g and a coercivity of approximately 2.01 Oe. In conclusion, adding Nb to the Fe-based alloy system improved its soft magnetic and thermal properties without compromising its amorphous characteristics. Furthermore, annealing further enhanced the magnetic properties.

**Keywords:** Soft magnetic, Nanocrystalline, Amorphous, melt-spinning, glass-forming ability

| P-H0647 |

# Reinforcement of Soft Magnetic Properties by Heat Treatment in Melt-spun Fe-based Ribbons

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## Abstract

The demand for efficient electric devices with exceptional soft magnetic properties has driven the exploration of Fe-based amorphous and nanocrystalline materials. Fe-based alloys are popular nanocrystalline alloys known for their high saturation magnetic flux density (Bs). However, there is a need to improve the amorphous forming ability (AFA) of Fe-based alloys known to have limitations in AFA. To address this, we introduced carbon to the Fe-based alloy to enhance AFA without compromising key characteristics such as high saturation magnetic flux density (Bs), low coercive force (Hc), and cost-effectiveness in manufacturing process. Our approach involved preparing ingots using both induction and arc melting techniques. These ingots were then transformed into melt-spun ribbons using the melt-spinning method, which employed a rotating copper wheel for rapid quenching. Heat treatment was conducted by annealing the ribbons at various temperatures for 10 minutes in argon atmosphere. Detailed analysis was conducted to evaluate the structural, magnetic, mechanical, and thermal properties of the ribbons. This analysis utilized equipment including an x-ray diffractometer (XRD), vibrating sample magnetometer (VSM), nanoindenter, differential scanning calorimeter (DSC), and magneto-optical Kerr effect microscope (MOKE). The annealed Fe-based ribbons demonstrated significant improvements in its magnetic properties, particularly an increase in saturation magnetic flux density from 1.62 T to 1.81 T, accompanied by low coercive force. These results mean the successful reinforcement of AFA in the Fe-based alloy system through carbon addition while preserving its excellent soft magnetic properties.

**Keywords:** Soft Magnet, Heat Treatment, Fe-based, Melt-spinning, Magnetic Property

# Tailoring the magnetic properties of Sm-Co nanocomposites through morphological evolution via HCl washing

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**Abstract.**

Magnetic materials having essential magnetic anisotropy and magnetization are being utilized for applications in various fields such as magnetic sensors and storage media. Therefore, in the present work, the one – dimensional SmCo nanocomposites were prepared using hydrazine reduction method. The samples are prepared in the presence of static magnetic field. The effect of post-synthesis washing of nanocomposites with diluted hydrochloric acid on the structural, morphological and magnetic properties is investigated through XRD: X-ray diffraction, HRFESEM- High resolution field emission scanning electron microscopy, EDS: Electron diffraction X-ray Spectroscopy and dc-magnetization. The XRD patterns revealed the formation of Sm-Co nanocomposites studied via Rietveld refinement procedure. The effect of HCl washing on the morphology of the nanocomposite was clearly visible demonstrating flower like structures. The major contribution of Sm and Co was observed in the EDS spectra. The magnetization vs magnetic field curves revealed ferromagnetic behavior along with a high value of saturation magnetization ~ 150 emu/g.

**Keywords:** One-dimensional Sm-Co Nanocomposites, Flower-like Morphology, Magnetic Anisotropy, dc-magnetization.

| P-H0987 |

# Approach to improve the MHz performance of Fe-Si based soft magnetic composites

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## Abstract

Improving MHz performance of soft magnetic materials is a key issue of efficient conversion for electric energy with high power level. However, low cut-off frequency of Fe-Si based soft magnetic composites limits their application in MHz frequency range in which the wide bandgap semiconductors can release full potentials. By decreasing Fe-Si particle size from 116 μm to 24 μm, the cut-off frequency of composites increases from 8 MHz to 110 MHz, and power loss decreases at 1 MHz clearly. Combining with the classical loss separation theory, it shows the decrease of particle size mainly supresses the loss of eddy current in particles. By increasing aspect ratio of particles, it is found the cut-off frequency increases further, while the loss of eddy current and excess loss decreases constantly. These shows MHz permeability comes from nature resonance modulated by the eddy current. Obviously, Weakening the eddy current is an effective way to increase the cut-off frequency of soft magnetic composites. This result has significance for release the potential of wide bandgap semiconductors.

**Keywords:** Cut-off frequency, Loss, Eddy current, Soft magnetic composites, Fe-Si

| P-H1181 |

# Characterization of Fe-6.5% Si steel sheet produced 3D Printing

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## Abstract

We investigated the characteristics that appear when making sheet-type Fe-6.5%Si steel that can be laminated through 3D printing, unlike existing bulk materials. Fe 6.5%Si powder was melted and polished by 3D printing to form a thin sheet of 0.35 mm, and then heat treated at 10-4 torr at 1150 degrees for 1 hour. As a result, stress was removed and a 500um columnar grain structure with like cube fibers was secured. And at a high frequency of 10,000h, it showed superior magnetic properties compared to commercial non-oriented electrical steel sheets. This result has enormous potential in the manufacture of a 6.5% si steel sheet form that can be stacked using 3D printing.

**Keywords:** 3d printing, steel, magnetic properties, electrical steel

| P-H1183 |

# Study on Moisture Trigger Self-Healing Effect of $Ti_3C_2T_x$ MXene Electrode with Application

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Two-dimensional (2D) materials composed of a single or several layers with a thickness of a few nanometers have been extensively studied in various field due to their unique properties such as flexibility, transparency, and electrical conductivity. E-skin is a flexible electronic device that can be attached to the skin or integrated into clothing to monitor health information and environmental factors such as temperature, pressure, and humidity. However, due to its flexible and smooth nature, e-skin is prone to damage and wear over time. Therefore, it is crucial that the accessory parts used in e-skin exhibit flexibility and smoothness, and that they are composed of materials capable of self-healing from damage caused by motion, to enhance the lifespan and durability of the device. Among the various 2D materials, Ti3C2Tx MXene have been identified as potential candidates for self-healing electrodes required by the e-skin field. The self-healing effect of Ti3C2Tx MXene has been demonstrated in several studies, but typically requires high heat or additional substances as triggers. However, these mechanisms are not suitable for devices that come into direct contact with the body, such as e-skin. As a result, a study was conducted to investigate the potential of using moisture as a trigger for self-healing in MXene, given the material's rich hydrophilic functional group on its surface. The findings suggest that self-healing at room temperature using only water without any additional additives could be a practical solution for incorporating MXene into e-skin technology in the future.

**Key word:** $Ti_3C_2T_x$ MXene, Self-Healing, E-skin, Moisture trigger, 2D materials.

# POSTER Session 1

## Symposium I : Biomaterials and Soft Materials and their Application

**P-I0102** **Functional and Hierarchical 3D Printed Scaffolds for Bone Tissue Engineering using 3Y-TZP/HAp Composites**
Tejas Mahesh Koushik (James Cook University, Australia)

**P-I0294** **Effect of Ni and Fe content on microstructure and mechanical properties of biomedical Co-Cr-Fe-Ni-Mo alloy**
Kai Hiyama (Tohoku University, Japan)

**P-I0401** **Flexible and transparent thermochromic device for energy-efficient smart windows using cellulose nanostructures**
Jae Gyu Ahn (Kongju National University, Korea)

**P-I0402** **Hierarchical nanostructure with high uniformity in pore size derived from balsa wood for electrochemical capacitors**
Taeyoung Park (Kongju National University, Korea)

**P-I0408** **Excellent CO2/CH4/N2 Adsorption Capacity and Selectivity for 3D Graphene Nanostructure derived from Cellulosic Biomass**
BeomJin Ko (Kongju National University, Korea)

**P-I0455** **Self-expandable Electrode based on Chemically polished Nickel-titanium alloy wire for Treating Endoluminal Tumors using Bipolar Irreversible Electroporation**
Song Hee Kim (University of Ulsan College of Medicine, Korea)

**P-I0573** **Endothelial cell behavior on pulsed-anodized NiTi alloys using different electrolytes**
Yuya Matsui (Kitami Institute of Technology, Japan)

**P-I0609** **Self-assembled bioactive inorganic core/chitosan shell nanounits doped biocomposite structure for applying therapeutic tissue engineering**
YoungEun Choe (Dankook University, Korea)

**P-I0725** **Optimized Manufacturing Processes for Low-cost High-performance Titanium Alloys: Controlling Beta Stability with Mo and Ferrochrome Contents**
Suhyun Oh (Korea Institute of Materials Science, Korea)

**P-I0778** **Effects of RBM, SLA, and PEO coating methods on the Fatigue Characteristics of the Dental Implant.**
Dr. Sidra Sadaf Nisar (Chosun University, Korea)

# POSTER Session 1

**P-I0779** **Comparing the Mechanical, Bio-corrosion, and Bio-compatibility of the surface-modified novel Ti-29Nb-5Zr and Conventionally Manufactured Ti-6Al-4V for dental implant applications**
ARUN S (Chosun University, Korea)

**P-I0870** **Design of Immune Suppressive Chitosan Hydrogel with Bioactive Molecule Conjugation**
Gyeongwoo Lee (University of Tsukuba, Japan)

**P-I0886** **Defining roles of the cathodic phase on the binary Mg alloys for the generation behavior of reactive oxygen species**
Minjung Chae (Korea Institute of Science And Technology, Korea)

**P-I0894** **Evaluation of bone fusion capability of interface free HA PEEK cage**
Minseong Chae (University of Ulsan, Korea)

**P-I0953** **Magnesium coated nerve conduit as a promising biomaterial for enhancing peripheral nerve regeneration**
Hyewon Kim (Korea Institute of Science And Technology, Korea)

**P-I0961** **Nanoparticle Based Platform for Rapid and Ultrasensitive Nucleic Acid Detection**
Sunyeoung Na (Hanyang University, Korea)

**P-I0965** **Ring-type, wearable blood pressure monitoring device capable of cuff-based measurement**
Minjoo Lee (Kwangwoon University, Korea)

**P-I0966** **Endotoxin-Free High Concentration M13 Bacteriophage for Biomaterial Applications**
JiHyae Choo (Hanyang University, Korea)

**P-I0976** **Plasma polymerized bio-interface directs fibronectin adsorptionto enhance "epithelial barrier structure" formation via FN-ITG β1-FAK-Mtor signaling cascade for the advancement of transepithelial metal impalnt**
Zhuofan Chen (Sun Yat-sen University, China)

**P-I0992** **Potential of M13 Bacteriophage as a Bio-Supercapacitor**
Yujin Lee (Hanyang University, Korea)

**P-I0997** **Battery-free wireless skin hydration sensor with breathable and low irritation**
Hyejun Kim (Kwangwoon University, Korea)

**P-I1025** **Customization of supramolecular hydrogels through one-step photopolymerization and its mechanism**
Ruifen Tang (Beijing University of Chemical Technology, China)

| P-I0102 |

# Functional and Hierarchical 3D Printed Scaffolds for Bone Tissue Engineering using 3Y-TZP/HAp Composites

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## Abstract

Bone tissue engineering (BTE) is an exciting and rapidly evolving field of research that holds immense promise for patients suffering from bone injuries or diseases. Recently, advances in materials science and our understanding of the bone healing process have opened up new possibilities for creating effective BTE scaffolds. The key challenge in designing synthetic scaffolds for BTE is balancing the need for load-bearing capability with the requirement for promoting interaction with the local extracellular matrix (ECM) to facilitate bone healing. However, by leveraging the power of additive manufacturing (AM) techniques, complex scaffold designs can be designed to meet these dual responsibilities.

In this paper, we take a closer look at the potential of bioceramics in AM strategies for BTE applications. We will introduce strategies to process multiple materials using ceramic 3D printing. In-vitro performance of composite BTE scaffolds of 3Y-TZP – Hydroxyapatite with triply modified minimal structures (TPMS) will be studied. Relationships between the scaffold architecture (TPMS structure and porosity), mechanical performance and bone healing ability will provide a framework for development of personalized scaffolds that are tailored to the specific needs of individual patients, offering better outcomes, and reducing the risk of complications.

The high resolution of stereolithography-based ceramic printing allows for the introduction of hierarchical structures that meet the mechanical requirements of the patient. By combining different materials and structural features, engineers can create unique scaffolds that possess specific bone healing and structural capacities, moving away from the traditional one-size-fits-all approach to a more personalized approach to BTE.

**Keywords:** Additive manufacturing, Bioceramics, Composites, Bone tissue engineering

| P-I0294 |

# Effect of Ni and Fe content on microstructure and mechanical properties of biomedical Co-Cr-Fe-Ni-Mo alloy

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## Abstract

A 40Co-20Cr-16Fe-15Ni-7Mo alloy (mass%, ASTM F1058, Elgiloy) is used in balloon-expandable stents because of its excellent mechanical and corrosion properties. Balloon-expandable stents with smaller diameter benefit minimally invasive medical treatments, which require both high strength and ductility of the alloys while keeping the corrosion resistance intact. We studied the effect of heat treatment on the microstructure and mechanical properties of this alloy[1]. In the present study, we investigated the effect of Ni and Fe on microstructure and mechanical and corrosion properties of Co-Cr-Fe-Ni-Mo alloys.

The chemical compositions of the alloys used in this study are (55–x)Co-20Cr-15Fe-xNi-7Mo-2Mn-0.08C (mass%, x=0, 5, 10, 15) and (55-y)Co-20Cr-yFe-15Ni-7Mo-2Mn-0.08C (mass%, y=0, 5, 10, 15). These alloys, referred to as (55-x)CoxNi and (55-y)CoyFe, were prepared using an induction melting furnace. As-cast alloys were subjected to hot forging and subsequent solution treatment. Solution-treated alloys were cold swaged, followed by heat treatment at 1273 to 1323 K. The microstructure was analyzed using EBSD. Mechanical and corrosion properties were evaluated by tensile testing and anodic polarization tests in Hanks' solution, respectively.

Recrystallization was observed in all heat-treated alloys. In the (55-x)CoxNi alloys, the ductility decreased with decreasing Ni content. The 50Co5Ni alloy exhibited TRIP-like work-hardening behavior, although its ductility was lower than that of the 40Co-20Cr-16Fe-15Ni-7Mo alloy. The ultimate tensile strengths were above 1000 MPa for all (55-y)CoyFe alloys. No significant differences in the anodic polarization curves of the (55-x)CoxNi alloys were observed.

## References

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Keywords: Co-Cr alloy, Elgiloy, biomaterials, stent, corrosion resistance

| P-I0401 |

# Flexible and transparent thermochromic device for energy-efficient smart windows using cellulose nanostructures

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## Abstract

Using eco-friendly, transparent cellulose-based wood as an alternative to existing interior materials can reduce indoor energy consumption and unsustainable construction waste while providing privacy. This study demonstrates an eco-friendly and cost-effective approach to creating flexible, transparent thermochromic devices for energy-efficient smart windows. The transparency of these devices can be easily adjusted not only by the thickness of the film but also by changing the composite ratio of UV curable polymers to liquid crystals. A composite film with a transmittance of 35% at room tempaerature and 79% at 80 °C is produced by combining UV curable polymer dispersion liquid crsytal (PDLC) and transparent wood (TW). It has a lower thermal diffusion rate (0.07mm2/s) than glass. In addition, these composite films have a realtively high transmittanc of 76% compared to TW using epoxy, showing a similar Young's Modulus (1.9~2.6 GPa). The unique and highly desirable properties demonstarated by thermochromic TW-PDLC films make energy-efficient smart windows a promising candidate for practical use.

**Keywords:** Transparent wood, Smart window, PDLC, Thermochromic, Energy-efficient

| P-I0402 |

# Hierarchical nanostructure with high uniformity in pore size derived from balsa wood for electrochemical capacitors

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## Abstract

Activated carbons derived from biomass resources with high micro- and meso-porosity are becoming increasingly popular for various applications, such as removing liquid and gas-phase pollutants and energy storage systems. Despite their significant advantages, the low uniformity of pore size and mass production challenges still hinder their use as electrodes in energy storage applications. In this study, we propose a cost-effective and scalable method to generate a graphene-based 3D nanostructure with a large specific surface area and highly uniform pore sizes through sequential delignification, carbonization and activation processes. We also evaluated the electrochemical characteristics of these structures as active materials in an electrochemical double layer capacitor. Textual and chemical analyses revealed a 3D network architecture comprising interconnected lamellar structures made of graphene sheets. These structures displayed high uniformity of nanoporosity and high electron conductivity. Furthermore, the electrochemical performance of the as-prepared materials exhibited a significant improvement of performance such as capacitance and cycling stability without any attenuation of capacitance. This enhancement can be attributed to the optimal porosity of the graphene-based 3D nanostructure, which increases ion access rates and provides more electron pathways onto the electrode. Our approach has potential applications in sustainable energy storage systems for practical implementations.

**Keywords:** 3D structure, Biomass, Capacitor, Activated carbon, electrical energy storage

| P-I0408 |

# Excellent $CO_2/CH_4/N_2$ Adsorption Capacity and Selectivity for 3D Graphene Nanostructure derived from Cellulosic Biomass

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## Abstract

Activated carbons have been known for their excellent gas adsorption properties, but their efficacy in powder form is compromised due to uneven particle size and porosity. In this study, we demonstrate a practical and eco-friendly method for producing uniform and highly porous 3D graphene nanostructures from wood-based biomass. The process involved delignification, carbonization, and activation steps. The adsorption capacity and selectivity of these structures for CO2, CH4, and N2 gases, as well as their performance in binary gas mixtures, were assessed. Our scientific and chemical analyses revealed that balsa wood has a layered structure interconnected by cellulose-based fibers following the delignification process. Additionally, we confirmed that the activated carbon in this experiment formed a 3D network similar to graphene with a large specific surface area (~ 1380 m2/g) and uniform micro-porosity ranging from 7-10 Å. The resulting 3D graphene network significantly enhanced the adsorption capacity of CO2, CH4, and N2 gases, and showed clear selectivity in binary gas mixtures. The experimental data for both pure gas and binary mixtures fit well with the ships isotherm model. Our results suggest that this biomass-derived 3D structure holds potential as a monolithic adsorbent for gas separation applications.

**Keywords:** Graphene, Carbon dioxide capture, Methane, Porous structure, Biomass

| P-I0455 |

# Self-expandable Electrode based on Chemically polished Nickel-titanium alloy wire for Treating Endoluminal Tumors using Bipolar Irreversible Electroporation

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## Abstract

The application of irreversible electroporation (IRE) to endoluminal organs is being investigated; however, the current preclinical evidence and optimized electrodes are insufficient for clinical translation. Here, a novel self-expandable electrode (SE) made of chemically polished nickel-titanium (Ni-Ti) alloy wire for endoluminal IRE is developed in this study. Chemically polished heat-treated Ni-Ti alloy wire demonstrate increased electrical conductivity, reduced carbon and oxygen levels, and good mechanical and self-expanding properties. Bipolar IRE using chemically polished Ni-Ti wires successfully induces cancer cell death. IRE-treated potato tissue shows irreversibly and reversibly electroporated areas containing dead cells in an electrical strength-dependent manner. In vivo study using an optimized electric field strength demonstrate that endobiliary IRE using SE evenly induces well-distributed mucosal injuries in the porcine common bile duct (CBD) with the overexpression of the TUNEL, HSP70, and inflammatory cells without ductal perforation or stricture formation. This study demonstrates the basic concept of the endobiliary IRE procedure, which is technically feasible and safe in a porcine CBD as a novel therapeutic strategy for malignant biliary obstruction. SE is a promising electrical energy delivery platform for effectively treating endoluminal organs.

**Keywords:** Irreversible electroporation, Nickel-titanium alloys, Chemical polishing, Self-expandable metallic stents, Electrode

| P-I0573 |

# Endothelial cell behavior on pulsed-anodized NiTi alloys using different electrolytes

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## Abstract

Pulsed anodization of NiTi alloy is surface modification process that overcomes drawbacks associated with biomaterial application. In the pulsed anodization, the chemical reaction between the oxide layer and the electrolyte is highlighted during a voltage off periods since the anodic reaction is suspended. Such mechanism enables the removal of Ni content in the surface, leading to the growth of an almost Ni-free TiO2 layer. As a result, the alloy surface is hydrophilized and further, the Ni ions release from the alloy is minimized. Obviously, the chemical reaction desrived by the electrolytes is key factor predominating the pulsed anodization, influencing to the layer properties relating with biocompatibility. Based on above, in this study, a NiTi alloy was pulsed-anodized in four types of electrolytes such as HNO3, H2SO4, NH4NO3 and (NH4)2SO4, and the surface characteristics and the endothelial cell behavior on the surface were evaluated. Using the H2SO4 electrolyte resulted in the formation of oxide layer with submicrometer roughness, on which cell morphology seemed to be compacted. A TiO2 layer with relatively smooth surface, yet cell proliferation was insufficient due to the increase of Ni ion release. Other two electrolytes, NH4NO3 and (NH4)2SO4, formed the similar smooth layer with the minimization of Ni ion release, thereby showing an extended cell morphology and high cell proliferation rate. In conclusion, the electrolyte selection is the significant factor to achieve a biocompatible surface on NiTi alloy via pulsed anodization; harein, NH4NO3and (NH4)2SO4 formed a better layer on a NiTi alloy surface.

**Keywords:** NiTi alloy, pulsed-anodization, endothelial cell, surface morphology, Ni ion release

Poster Session 1

| P-I0609 |

# Self-assembled bioactive inorganic core/ chitosan shell nanounits doped biocomposite structure for applying therapeutic tissue engineering

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## Abstract

Natural inorganic/organic nanohybrids have been extensively used in biomaterials design as they can provide extraordinary properties (e.g., nanotopography and multiple-therapeutic delivery), to successfully accomplish cellular activation. In this study, we propose a new strategy for fabricating unique structured nanohybrids through self-assembly of biomedical inorganic/organic nanounits. These nanohybrids were able to load multiple therapeutic molecules in the core and shell compartment and then release sequentially, demonstrating controlled delivery systems. To obtain these unique nanohybrids, we selected two different core/shell nanounits; i) hydroxyapatite (HA) and phenamil in core/chitosan in shell nanounit and then ii) trichostatin A (TSA) in core/gelatin in shell nanounit. To show the efficacy of these therapeutic nanohybrids as hard tissue engineering platform, these nanohybrids were sequentially coated on the fabricated 3D printed PCL/HA scaffolds. As results, the nanohybrids compartmentally-loaded with therapeutic molecules (TSA and phenamil) were shown to stimulate the anti-inflammatory, pro-angiogenic, osteogenic, and epigenetic events of relevant cells. The nanohybrids coated constructs presented a higher degree of osteogenic activity than the control, which was fabricated using normal printed hydrophobic PCL/HA and NaOH treated hydrophilic PCL/HA scaffolds. Thus, the proposed nanohybrids self-assembled from nanounits can be a promising use of 3D tissue engineering scaffold platform for applying therapeutic bone tissue regeneration.

**Keywords:** Self-assembly, Inorganic/organic nanohybrids, Controlled drug delivery, Tissue regeneration

| P-I0725 |

# Optimized Manufacturing Processes for Low-cost High-performance Titanium Alloys: Controlling Beta Stability with Mo and Ferrochrome Contents

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Titanium alloys, with its high strength-to-weight, excellent corrosion resistance, and biocompatibility, is finding expanded applications in various industries such as aerospace, marine, energy, chemical and medical industries. Beta titanium alloys, in particular, exhibit superior workability compared to other alloys, enabling them to be utilized in a wide array of medical and consumer sectors such as biomedical implants, eyeglass frames, and sports and leisure equipment. However, conventional beta titanium alloys often contain costly alloying elements, including Nb, V, and Zr, which impose economic constraints. Moreover, the microstructure of titanium alloys, which significantly influences their mechanical characteristics, is determined by thermo-mechanical processing, emphasizing the need for optimized manufacturing processes.

In this study focuses on selecting Mo, a relatively cost-effective beta stabilizing element, as the primary alloying element, and incorporating low-cost ferrochrome to enhance the low strength of Ti-Mo binary alloys. The beta stability is controlled by varying the amounts of Mo and ferrochrome. The alloys are produced through a thermo-mechanical treatment such as hot rolling and solution treatment to induce the formation of the α'' phase. Subsequent cold rolling treatment is applied for the development of [100] texture, resulting in characteristics of low modulus, high strength and optimizing the manufacturing process of high-performance titanium alloys.

| P-I0778 |

# Effects of RBM, SLA, and PEO coating methods on the Fatigue Characteristics of the Dental Implant.

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## Abstract

The functionality and stability of the implant and the implant-bone interfaces serve as crucial factors for the assessment of a dental implant's long-term success. Although, dental implants' success is influenced by a number of variables, one of the most decisive is better fatigue fracture resistance. Therefore, the study aimed to examine the effects of resorbable bone media (RBM), SLA (sandblasted and acid-etched), and PEO (plasma electrolytic oxidation) coating methods on the fatigue characteristics of dental implants using a fatigue tester machine (Instron) under 80%, 60%, and 40%, and 23% loads as calculated using the maximum static load of 1082 N. To examine the fatigue characteristics, the fixture, abutment, and metal caps were prepared using a Ti-6Al-4V alloy, and the coating process of RBM, SLA, and PEO was done on the abutment screw for analyzing the fatigue strength. After undergoing 80%, 60%, 40%, and 23% loads of the maximum load of 1082 N then the fracture surfaces were observed by field-emission scanning electron microscopy (FE-SEM; S-4800, Hitachi, Japan) and energy dispersive X-ray spectroscopy (EDS; S-4800, Hitachi, Japan).

**Keywords:** RBM, SLA, PEO, Coating methods, Fatigue resistance, Dental implant
Acknowledgment: This research was supported by NRF (2021R1A4A1030243; 2023R1A2C1005748; RS-2023-00222390).



Fig. 1. Fixture, abutment, fixing screw, and metal cap.

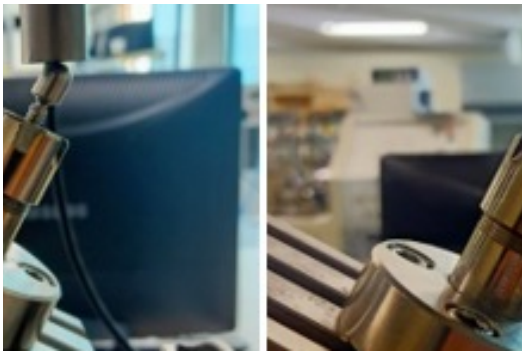


Fig. 2. The experimental instrument and cyclic loading of bulk (uncoated) sample.

| P-I0779 |

# Comparing the Mechanical, Bio-corrosion, and Bio-compatibility of the surface-modified novel Ti-29Nb-5Zr and Conventionally Manufactured Ti-6Al-4V for dental implant applications

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The advantageous properties of Titanium (Ti) and Ti alloys over other metallic biomaterials render them the primary design choice for biomedical applications. The surface modification of the Ti is important as it plays a crucial role in determining the service life of the implant system. The present work aims to evaluate the performance of the oxide layer formed on the novel Ti-29Nb-5Zr and conventional Ti-6Al-4V alloy by the plasma electrolytic oxidation process (PEO). The PEO was carried out in an optimal coating condition in an electrolyte containing Ca/P with various concentrations of metallic ion additives such as Ag, Zn, Mn, and Mg. The effect of metal ion doping on the physiochemical properties of the different coated systems was investigated. Further, the effect of dopants in the anatase to rutile transformation rate also was studied in detail. The nano-mechanical properties of the coatings were evaluated using Vickers nanoindenter. The bio-corrosion test was done on the coated system using the electrochemical impedance spectroscopy technique in biological solution. The biocompatibility in terms of cell adhesion and cell proliferation of the coated system is studied using MC3T3-E1 cells. Based on the experimental findings, the PEO surface-modified newly developed Ti-29Nb-5Zr alloy is a promising material for dental implant applications. (This research was supported by NRF: 2021R1A4A1030243; 2023R1A2C1005748; RS-2023-00222390).

**Keywords:** Plasma electrolytic oxidation, Ti-29Nb-5Zr, Ti-6Al-4V, Nanoindentation, Biocompatibility.

# Design of Immune Suppressive Chitosan Hydrogel with Bioactive Molecule Conjugation

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## Abstract

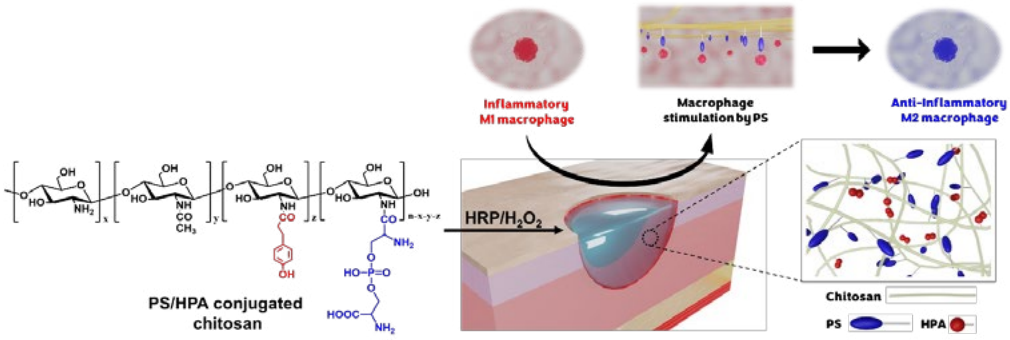
Background: Phosphoserine (PS) group is a natural immune suppressive biomolecule. It is a phospholipid head distributed on the inner cell layer and exposed to the outside by apoptosis the programmed cell death[1]. The exposed PS group suppresses the immune system by interacting with macrophage. In the inflammation tissue, the macrophage exists as an inflammatory phenotype M1 and mediates the inflammatory response by secretion of cytokine and other molecules. Through the interaction with PS group, M1 macrophage is polarized to the anti-inflammatory phenotype M2 and mediates the resolution of inflammation and tissue repair[2]. In this study, PS group was introduced to chitosan and fabricated to the hydrogel as an immune modulative novel material.

Method: To fabricate the PS conjugated chitosan hydrogel, the crosslink moiety phloretic acid (HPA) and protected PS group was introduced by EDC/NHS reaction and deprotected by hydrochloric acid. Synthesized polymer was fabricated to the hydrogel by enzyme/catalyst reaction. Synthesis of polymer, physical properties and physical properties of hydrogel were evaluated.

Results: The successful synthesis was observed in 1H NMR, and conjugated HPA and PS group was quantified by UV-vis and ICP-OES. Hydrogel was crosslinked within 30 seconds and showed soft mechanical property that is storage modulus around 200 Pa. Conjugation of PS group improved hydrophilicity of hydrogel without any adverse effects in terms of cell viability. Also, immobilized PS group suppressed immune response successfully.

**Reference:** [1] Fadok, Valerie A., et al., 5.7 (1998): 551-562. [2] Wu, Yu-Sheng, and Shiu-Nan Chen. Frontiers in pharmacology 5 (2014): 1.

**Keywords:** Biomaterial, Natural polymer, Hydrogel, Immune modulation




Scheme. Fabrication of PS/HPA conjugated hydrogel and polarization of macrophage.

| P-I0886 |

# Defining roles of the cathodic phase on the binary Mg alloys for the generation behavior of reactive oxygen species

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## Abstract

The corrosion products of biodegradable metals such as hydrogen gas (H2) and reactive oxygen species (ROS) have been variously applied in the field of biomedical engineering. Here, we investigate the mechanisms of ROS generated by the corrosion of pure Mg, binary Mg-Ca alloy, and Mg-Zn alloy. The amount of ROS generation is determined by the relative position between the conduction band edge of the oxides formed on the the surface of cathodic phase and the redox potential of ROS. Among the various corrosion products from Mg-Zn alloy, ZnO has its conduction band edge slightly more positive than the superoxide anion redox potential, facilitating the transfer of electrons to dissolved oxygen to produce superoxide anions. The study suggests that an oxide coating on the biodegradable metal surface can control ROS generation, considering the conduction band position of oxides and ROS redox potential. This research provides insight into biomedical applications that induce or suppress ROS generation through surface design such as alloy manufacturing, surface coating, and surface treatment.

**Keywords:** Magnesium alloys, Galvanic corrosion, ROS, Corrosive mechanism, Biodegradability

| P-I0894 |

# Evaluation of bone fusion capability of interface free HA PEEK cage

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## Abstract

Polyetheretherketone (PEEK) is a widely accepted implantable material that has relatively higher strength and superior durability than other polymers. However, due to its bioinertness, PEEK is not able to integrate with bone tissue. Recently, a various bioactive coating was developed to improve bone-to-PEEK bonding ability.

Nevertheless, since the coating layer are easily peeled off during the procedure, research is continued to strengthen the interfacial bonding force of the coating layer. It was tried to overcome this drawback by using a specific process that involves the use of nanosecond lasers to synthesize interface-free HA/PEEK surface. The aim of this study was to prove bioactivity of the interface free PEEK cage in canine anterior cervical fusion model.

HA/PEEK cage (W10 x D6 x H4 mm) is a specimen treated to prevent the interface from being separated from HA with Interface free laser on both sides in contact with the residential bone. In three beagles, both interface free HA/PEEK cage and pure PEEK cage (control) were implanted into the cervical intervertebral space (C3/4 or C4/5) with auto graft. After the 12-weeks survival period, interbody fusion activity evaluated based on histology and histomorphometry by measuring new bone volume (NBV).

The NBV of interface free HA/PEEK cage group was found to be 40.04%, while the new bone volume of pure PEEK cage group was only 13.57%. The new bone volume (%) was significantly greater for interface free HA/PEEK cage group than for the pure PEEK cage group (showing a 26.47% difference; $p<0.005$).

**Keywords:** PEEK, HA coating, Cervical cage, Bone fusion, Bone reconstruction

| P-I0953 |

# Magnesium coated nerve conduit as a promising biomaterial for enhancing peripheral nerve regeneration

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## Abstract

Biodegradable magnesium is highlighted in medical applications, with magnesium ions showing the potential for enhancing nerve regeneration. However, their uncontrollable biodegradation is a difficult challenge to overcome. Bio-functional based nerve conduit is a promising strategy to promote nerve regeneration. Here, we developed a novel system that can effectively control magnesium biodegradation by sputtering magnesium onto biocompatible collagen sheets. The newly developed system facilitates faster and longer neurite outgrowth and exhibited excellent cell viability by promoting the differentiation of neuronal precursor cells. Moreover, we performed the implantation of magnesium-coated nerve conduits in 10mm nerve defects to evaluate the axon regeneration, remyelination, and functional recovery analysis at 12 weeks post-operation. In conclusion, our strategy suggests an interesting new way to facilitate the repair of challenging peripheral nerve injuries.

**Keywords :** Magnesium, nerve conduit, biomaterial, peripheral nerve regeneration

| P-I0961 |

# Nanoparticle Based Platform for Rapid and Ultrasensitive Nucleic Acid Detection

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## Abstract

Recently, detection methods targeting nucleic acids via DNA-functionalized nanoparticles have gained much attention with higher sensitivity and more rapid detection than traditional PCR (polymerase chain reaction). We developed a PCR-based molecular diagnostic system termed nSLAM (nanoparticle-based Surface Localized AMplification), which detects target nucleic acids using Fe3O4 (core)–Au (shell) nanoparticles (CSNPs). The CSNP surface is functionalized with oligo primers that are complementary to the target nucleic acids. These primers directly participate in the amplification process and function to accumulate and collect amplicons on the nanoparticle surface, thereby showing amplification efficiency enhancement.

The amplicons are converted into electrical signals through ECD (electrochemical detection), which are used to verify the presence of target nucleic acids. In the nSLAM system, the CSNPs act as dispersible electrodes and facilitate the transfer and contact of target nucleic acids towards the working electrodes. As a result of repetitive ECD measurements, signals are significantly amplified enabling highly sensitive molecular diagnosis.

To evaluate the detection performance, we used WHO-recommended primer sequences and three different nucleic acid targets (N2, E, RdRP gene) from the SARS-CoV-2 wild type genome. With 35 amplification cycles, the nSLAM system was able to detect a concentration of at least 1 RNA copy/μL. Furthermore, the number of amplification cycles were reduced to as low as 4 cycles (about 7 minutes) using 1 fM concentration cDNA. This demonstrates that the nSLAM system can reduce the lengthy runtime needed to detect SARS-CoV-2 via traditional PCR. The nSLAM system is a promising solution for early response of future pandemics through the rapid and ultrasensitive screening of pathogens.

**Keywords:** DNA-functionalized nanoparticles, gene amplification, electrochemical detection, nucleic acid biosensor, molecular diagnosis

| P-I0965 |

# Ring-type, wearable blood pressure monitoring device capable of cuff-based measurement

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## Abstract

The increasing mortality rates associated with cardiovascular diseases have highlighted the importance of real-time blood pressure monitoring for disease prevention and management. For blood pressure monitoring, non-invasive blood pressure measurement methods provide convenience. One of the non-invasive blood pressure measurement methods, photoplethysmography (PPG)-based method offers portability and ease of attachment, enabling convenient real-time blood pressure monitoring. However, when PPG is used alone, accuracy can be compromised due to factors such as noise, weak pulsations, and non-pulsatile components. On the other hand, automatic non-invasive blood pressure (ANIBP) measurement method based on oscillometry provides relatively higher accuracy by using cuff. But this method is less suitable for real-time monitoring and portability. To overcome these limitations, this paper introduces a soft, small-sized ring-shaped device that combines a PPG sensor with a pressure sensor, presenting a novel approach to blood pressure measurement. While several studies have investigated improving blood pressure measurement accuracy by using PPG with electrocardiography (ECG) sensor or developing signal analysis techniques, our device integrates the principles of cuff-based blood pressure measurements with PPG. To apply pressure, the device utilizes the user's usual movements without the need for a motor, resulting in more precise blood pressure measurements compared to PPG-based methods alone. Furthermore, this device is designed with considerations for comfort and wearability, featuring a small size and soft structure. Consequently, the platform proposed in this paper offers a more comfortable wearing experience and a higher level of accuracy by utilizing the cuff-based measurement compared to existing PPG single-technique applied monitoring devices.

**Acknowledgement**

This research was supported by the Basic Research Program through the National Research Foundation of Korea (NRF) funded by the MSIT (RS-2023-00222124).

**Keywords :** blood pressure measurement, photoplethysmography (PPG), cuff-based measurement, small size and soft structure, wireless real-time monitoring

| P-I0966 |

# Endotoxin-Free High Concentration M13 Bacteriophage for Biomaterial Applications

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## Abstract

M13 bacteriophage is a promising biomaterial for cell/tissue engineering based on the structural similarity with the ECM (extra cellular matrix) and the feasibility of chemical/genetic surface modification. Despite its advantages, intrinsic endotoxin contamination during production of M13 bacteriophage using Escherichia coli (E. coli) has been an issue, which quantitatively restricts the amount of material that can be used in bio/medical applications.

To solve this matter, we investigated a purification method using PEG-NaCl/Triton x-100 for preparing endotoxin-free (EF) high concentration M13 bacteriophage. Prior studies have used the Triton x-114-based endotoxin purification method, which uses phase separation for preparing low endotoxin level M13 bacteriophage. However, this method is unsuitable for producing high concentration EF M13 bacteriophage due to low yield. Thus, we adopted the PEG-NaCl/Triton x-100 method to purify large amounts and high concentrations of M13 bacteriophage. This purification method can produce endotoxin-free M13 bacteriophage pellets effectively without being damaged by solubilized endotoxins during PEG-NaCl precipitation due to the amphipathic property of the Triton x-100. We produced high concentration (~5 mg/ml, 1013 PFU) EF M13 bacteriophage and confirmed the efficiency of Triton x-100 endotoxin purification. Endotoxin removal levels were evaluated using the Limulus Amebocyte Lysate (LAL) assay, whereas the M13 bacteriophage damage during the purification process was assessed by plaque-forming assay and TEM imaging. Furthermore, in vitro-scale cytotoxicity and pro-inflammatory gene expression tests were conducted to confirm the biocompatibility of EF M13 bacteriophage.

These results show that our method can produce EF high concentration M13 bacteriophage efficiently, which can promote the use of M13 bacteriophage in cell/tissue engineering applications.

**Keywords:** M13 Bacteriophage, Endotoxin, Triton X-100, LAL Assay, Biomaterial

Poster Session 1

| P-I0976 |

# Plasma polymerized bio-interface directs fibronectin adsorptionto enhance “epithelial barrier structure” formation via FN-ITG β1-FAK-mTOR signaling cascade for the advancement of transepithelial metal impalnt

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## Abstract

Transepithelial metal implant, including transepithelial osseointegrated metal prosthetics (limbs, ears, dental implants, etc.), have drawn increasing interests for their convenience, efficacy and comfort of treatment. However, different with natural epithelial barrier, transepithelial interface-epithelial barrier is sustained by the inferior formation of “epithelial barrier structures”, thus have become the major risk factor causing infection and failure of epithelium-penetrating metal implants. How to increase the “epithelial barrier structures” (focal adhesions, hemidesmosomes, etc.) becomes one key research aim in overcoming this difficulty. Directly targeting the in situ “epithelial barrier structures” related proteins (such as fibronectin) absorption and functionalization can be a promising way to enhance interface-epithelial integration. Herein, we fabricated three plasma polymerized bio-interfaces possessing controllable surface chemistry. It is found that generated plasma polymerized surfaces could successfully direct distinguished protein adsorption profiles from serum protein pool, in which ppAA surface favors adsorbing adhesion related proteins and can promote FN absorption and functionalization via electrostatic interactions and hydrogen bonds, thus subsequently activating the ITG β1-FAK-mTOR signaling and promoting gingival epithelial cells adhesion. The study offers an effective perspective to overcome the current dilemma of the inferior interface-epithelial integration by in situ protein absorption and functionalization, which may advance the development of transepithelial metal impalnt.

**Keywords:** Transepithelial metal impalnt, Plasma polymerized bio-interface, Fibronectin adsorption, Epithelial barrier structure

| P-I0992 |

# Potential of M13 Bacteriophage as a Bio-Supercapacitor

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## Abstract

M13 bacteriophage possesses high potential to be used as a bio-supercapacitor due to its various traits such as adjustable electrical capacitance and easy production. M13 bacteriophage is a high-aspect-ratio fibrous phage with surface proteins that have an inner positive charge and outer negative charge, which are aligned along the axial direction of the phage. These surface proteins enable polarization of the phage, which can be maximized by unidirectionally aligning the materials in the same direction. We anticipated that this property could enable the use of the biomaterial as a capacitor, and thus, we subsequently conducted electric capacity measurements to confirm this idea. The electric capacity was proportional to the amount of aligned bacteriophage, whereas the unaligned bacteriophage could not serve as an electrode. Furthermore, the bacteriophage electrode showed great stability with negligible capacitance loss after repeated charge/discharge cycles and deformation tests. Therefore, these findings have identified the potential of M13 bacteriophage as a bio-supercapacitor, which we hope to be used as batteries for bio-transplant devices and electrodes for electrical signal transmission.

**Keywords:** M13 bacteriophage, biomaterial, supercapacitor.

| P-I0997 |

# Battery-free wireless skin hydration sensor with breathable and low irritation

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Recently, wearable biosensors capable of real-time monitoring have been widely used. Wearable sensors should be made light and thin to be comfortable to wear for a long time, and adhesives that can cause itching and skin irritation should be avoided for patients with sensitive skin. This paper describes developing a human-friendly biosensor using light and thin materials to accurately monitor skin dryness. Additionally, it enables patients to monitor skin dryness in real-time, as it is a direct factor affecting skin health. In this study, the following characteristics are obtained by using human-friendly materials and mesh materials. First, the light and thin sensor design enhances wearability and portability. The sensor is lightweight and has a thin construction that allows conformal contact with the user and puts no strain on the skin during daily activities. Second, the mesh material is highly breathable, allowing the skin to breathe naturally, preventing unnecessary moisture or heat. Soft skin contact provides a safe and comfortable fit even for users with sensitive skin. Thirdly, a special human-body-friendly coating minimizes skin interaction, increasing the accuracy and reliability of the sensor The special coating applied between the sensor and the skin is a human-friendly material that effectively transmits sensor signals without straining the skin. This allows users to wear it for extended periods of time and accurately monitor skin dryness. Lastly, the fusion of bio-sensing technology helps to accurately detect and judge skin dryness. Based on this, the sensor measures the amount of moisture in the skin in real time using bio-sensing technology to accurately determine the degree of skin dryness. This allows users to determine the dryness of an individual's skin and take necessary care measures. This sensor can be used in various fields such as medical, beauty, and sports that require skin monitoring.

**Acknowledgment**

This research was supported by the Basic Research Program through the National Research Foundation of Korea (NRF) funded by the MSIT (RS-2023-00222124).

| P-I1025 |

# Customization of supramolecular hydrogels through one-step photopolymerization and its mechanism

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## Abstract

Hydrogels used for different applications meet specific requirements of mechanical properties, leads to complicated materials and processes design. Here reports a simple one-step method for achieving a series of transparent hydrogels with highly tunable properties through free-radical photopolymerization (FRPP) of a single monomer, inspired by the fundamental mechanism of FRPP kinetics. The properties of poly-N-acryloyl 2-glycine (PNAG) hydrogels could be tailored within a range of 0.14 to 2.58MPa tensile strength, 15 to 519kPa Young's modulus, and 33 to 2.8*103g/g water-absorbing capacity by adjusting the polymer chain length and intermolecular interactions. The strongest PNAG hydrogel, with a tensile strength of 2.58 MPa, could be stretched to 14 times its original length and showed high elasticity with low hysteresis under cyclic loading at low deformation. More intriguingly, the photochemical decomposition rate of photoinitiator 1173 under UV-LED (365nm) and the internal interactions of PNAG hydrogels were found to be temperature-dependent, which may offer a promising supplement to the temperature effect theory in FRPP. This work not only presents a new perspective for the design of hydrogels for specific application but also paves the way for more extensive cooperation between FRPP with other preparation methods.

**Keywords:** Hydrogel, Free-radical photopolymerization, Temperature-dependent, Customization

# POSTER Session 1

## Symposium J : Materials Characterization and in situ/3D/4D Analysis

**P-J0457** **Hardness and wear properties of sintered Cu-Sn-Ni-Bi alloys**
Junhyub Jeon (Jeonbuk National University, Korea)

**P-J0484** **Micro probe system for in-situ x-ray scattering**
Soyeon Kim (Nextron Corporation, Korea)

**P-J0534** **Superplastic and ultra-high strength Si nanoparticles with oxide shell**
Wei Xu (Xi'an Jiao Tong University, China)

**P-J0572** **Room-temperature sintering-like agglomeration of diamond nanoparticles via ion irradiation**
Shaochuan Zheng (XI'AN JIAOTONG University, China)

**P-J0625** **Microstructural characterization of cost-effective Inconel 738LC while reducing expensive Co compositions**
Saurabh Tiwari (Gyeongsang National University, Korea)

**P-J0650** **Improved cryogenic tensile properties of additive manufacturing processed STS316L steel by the reusable powder**
Chohyeon Lee (Gyeongsang National University, Korea)

| P-J0457 |

# Hardness and wear properties of sintered Cu-Sn-Ni-Bi alloys

**Junhyub Jeon**[1], Namhyuk Seo[2], Ji-Woo Park[3], Seok-Jae Lee[4], Jae-Gil Jung[5], Min-Su Kim[6,†]

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## Abstract

Pb-containing Cu alloys have been widely adopted for various industrial applications such as bearings, shafts, or hydraulic pumps because of its apposite mechanical properties and self-lubricating effect. However, lead, which causes a self-lubricating effect, is detrimental to the environment and legally restricted in some countries. In the present study, the hardness and wear properties of Cu-Sn-Ni alloys containing different Bi contents were investigated to confirm whether Bi could be used as a substitute of Pb in Cu alloys to achieve favorable tribological performances. Cu-Sn-Ni-Bi alloys were fabricated by sintering the mixture of Cu-based powders, pure Ni powder, and pure Bi powder under vacuum condition at 850°C. Rockwell hardness and pin-on-disc tests were adopted to determine the hardness and wear properties of Cu-Sn-Ni-Bi alloys, respectively. Microstructures of the sintered alloys and their worn surfaces were examined by field-emission scanning electron microscopy. Phase identification was also conducted from X-ray diffraction analysis. It was observed that the hardness of sintered alloys had a tendency to increase as Bi content in the alloys increased. Also, the friction coefficients of the alloys tended to increase as Bi content increased.

**Keywords:** Cu-Sn alloy; Self-lubricating effect; Sliding material; Wear; Microstructure

| P-J0484 |

# Micro probe system for in-situ x-ray scattering

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## Abstract

Simultaneous electrical and structural measurements provide necessary information for dynamics of structural and electronic phase transition or modulation. In this poster, we would like to present a new platform of next-generation micro probe system, which combine functionality of conventional environmental-controlled micro probe system and x-ray scattering technique. The light weight and compact design are suitable for lab-based and synchrotron x-ray scattering experiments. In addition, it can easily create extreme environments: high temperature as high as 1000 oC, high vacuum as low as 0.9 x 10-4 Torr, and oxidizing/reducing condition with different gases. With an oxygen sponge SrFe0.8Co0.2Ox, the apparatus was tested in a lab x-ray diffractometer and a synchrotron-based diffractometer. Redox-driven structural change was clearly reproduced as demonstrated previously. In addition, simultaneous dc transport results clearly support associated modulation in its resistivity. Thus, the system can be applied not only for electrochemical experiments but also field-driven phase transitions in the controlled environments.

**Keywords:** Probe system, in-situ XRD, battery, SFCO

| P-J0534 |

# Superplastic and ultra-high strength Si nanoparticles with oxide shell

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## Abstract

Micro-nanoscale monocrystalline silicon is ubiquitous in many micro- and nanoscale technology applications, especially microelectronics and microelectromechanical systems (MEMS). However, despite their widespread use, issues related to their uncertain mechanical reliability remain a major factor hindering the further development of the device's commercialization. In particular, reliability issues related to MEMS component breakage are becoming increasingly important given the continued reduction in the size of key features, unexpected shocks during MEMS devices, and higher demands on harsh usage conditions. Understanding the mechanical behavior of silicon nanoparticles is important for the study of nanocontact between independent structures of silicon in MEMS systems. For example, fatigue and failure during the operation of mechanical components of MEMS can lead to the overall failure of the entire system. The improvement of mechanical properties such as strength, toughness and fatigue life of silicon structural parts is very important for the safe and stable operation of MEMS. Commercial silicon nanospheres are treated through a thermal oxidation process, and the heat-treated silicon spheres are coated with a smooth amorphous oxide film compared to the original oxide film surface. At the same time, by adjusting the heating temperature and heating time, we prepared the thickness of the amorphous oxide film with controllable thickness, and through the in-situ mechanical test of transmission electron microscopy, we found that the heat-treated silicon nanospheres, compared with the untreated commercial silicon nanospheres, the mechanical behavior changed from brittleness to plasticity, the strength was nearly doubled, and the plasticity was increased by nearly 5 times.

**Keywords:** Silicon, In situ mechanics, Nanospheres, Plastic, Strength

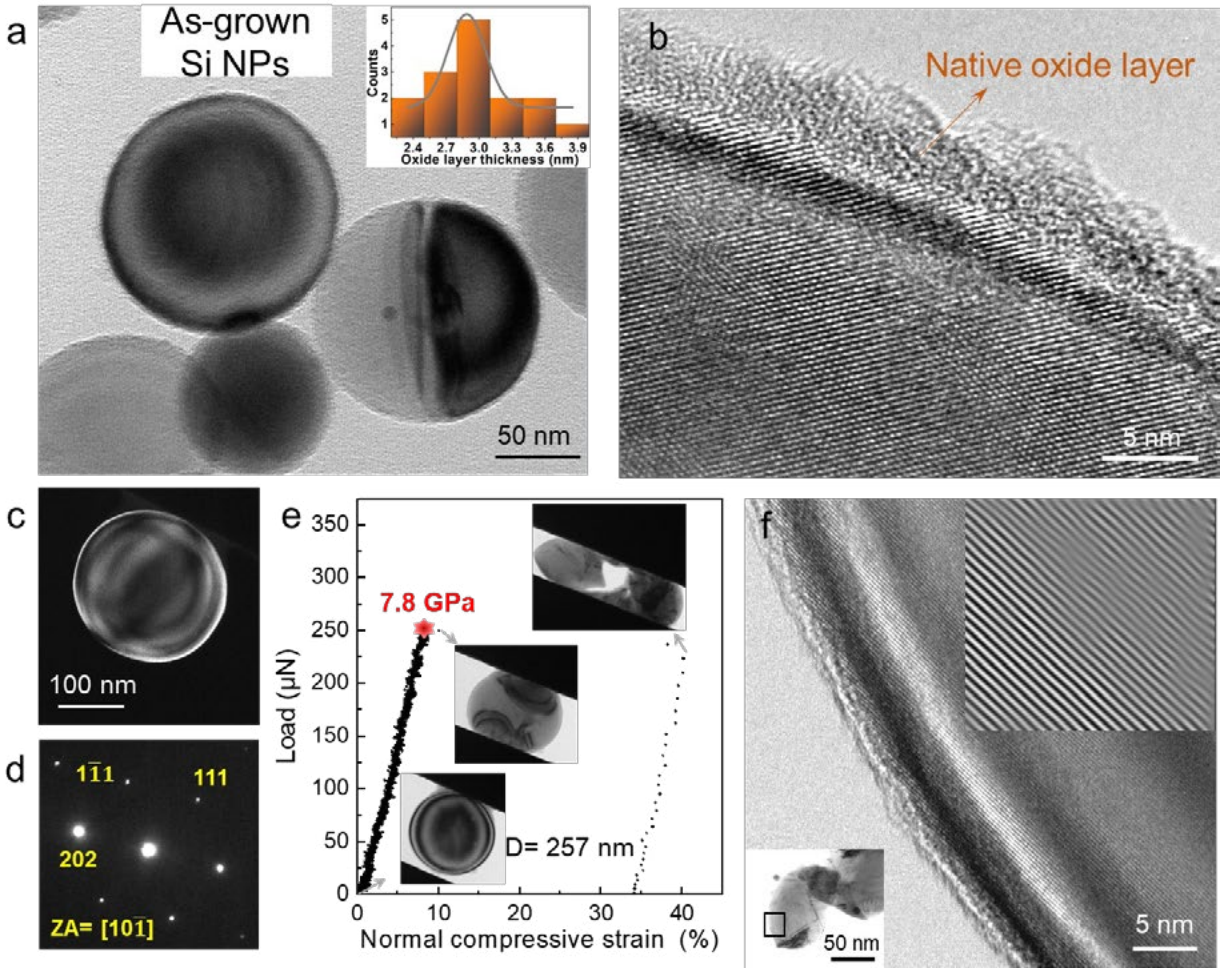



**Figure 1a.** Transmission electron microscopy image of silicon nanospheres (inset is a statistical chart of amorphous oxide film thickness) b. High-resolution image of transmission electron microscopy at amorphous oxide film of silicon nanospheres c. Darkfield image of silicon nanospheres d. Diffraction speckle image of silicon nanospheres e. Silicon nanospheres compression load-compression ratio relationship diagram (the inset is a screenshot of the compression process) f. High-resolution silicon nanospheres after compression (the inset are transmission electron microscopy image and FFT after compression)

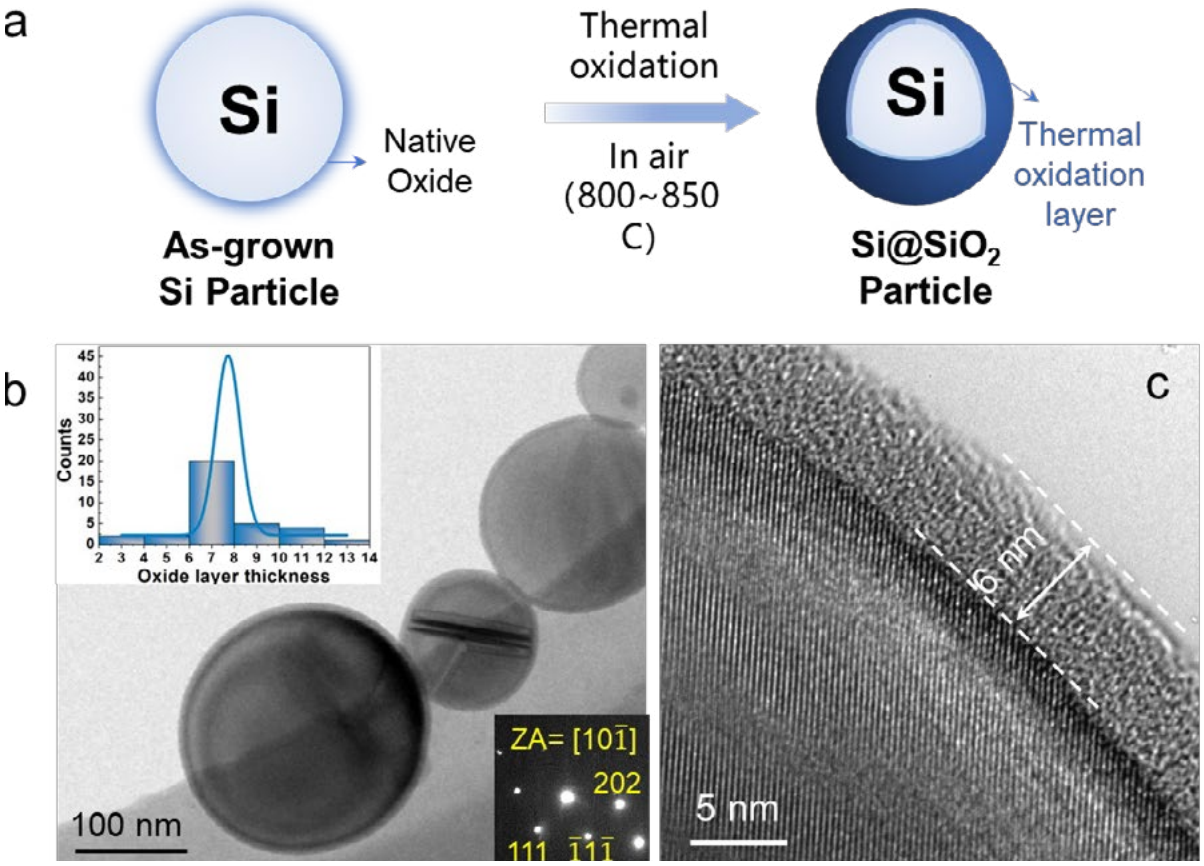



**Figure 2a.** Schematic diagram of the thermal oxidation process of silicon nanospheres b. Transmission electron microscopy image of thermal silica sphere (inset with amorphous oxide film thickness statistics and diffraction spot image) c. High-resolution image at an amorphous oxide film of thermal silicon oxide nanospheres

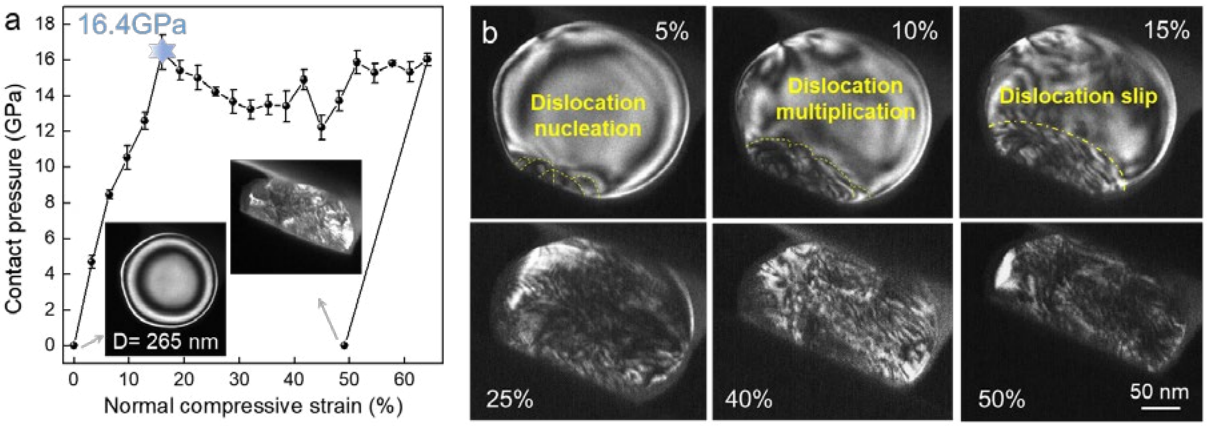



**Figure 3a**. Thermal oxide nanospheres compression contact stress-compression ratio diagram b. Screenshot of the darkfield compression process of thermal silicon oxide nanospheres

| P-J0572 |

# Room-temperature sintering-like agglomeration of diamond nanoparticles via ion irradiation

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## Abstract

With the development of synthetic nanodiamond particles, the investigation of the structural processing and surface modification of nanodiamonds under various conditions has been brought to the forefront. The SP3 chemical bond of diamond requires extremely high energy to break, such as high temperature and pressure. The traditional sintering process of nanodiamonds particles is carried out under ultra-high temperature and ultra-high pressure. It would seem counterintuitive that Sintering diamond grains together at room temperature, But through experiments, we found that the SP3 chemical bond of diamond can be converted to SP2 chemical bond by focusing ion beam at room temperature. Using in-situ microscopic as well as bulk experiments, here we demonstrate that quantitative irradiation of gallium ion beam can make nanodiamonds particles occuring the phenomenon of sintering. We can prove that the outer surface of sintered nanocrystalline diamond particles was coated with amorphous carbon via the result of electron energy loss spectroscopy (EELS). Nanodiamonds particles transform to amorphous from the surface, different particles were bonded together by the amorphous carbon. If a large number of nanodiamonds powders can be transform into sintered blocks by this method, we believe that under the premise that its strength can be guaranteed, the toughness will inevitably be greatly improved.

**Keywords:** nanodiamond; sintering; amorphous carbon; ion irradiation

| P-J0625 |

# Microstructural characterization of cost-effective Inconel 738LC while reducing expensive Co compositions

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## Abstract

Inconel 738LC has gained popularity in gas turbine applications due to its exceptional mechanical properties at elevated temperatures. However, the high cost of the substantial cobalt addition (8.00-9.00 wt%) limits its widespread use. In this study, we focus on reducing the cobalt content in Inconel 738LC while enhancing its tensile strength by 12% across various temperatures ranging from room temperature to 932 °C. The mechanical properties of the alloy are heavily influenced by the morphology and composition of Ni3(Al, Ti)-type precipitates (γ′). The characteristics of γ′ precipitates can be attributed to factors such as interface energy and γ/γ′ misfit. Therefore, our research aims to investigate the atomic-scale chemical composition changes in constituent phases, namely the γ matrix and γ′ precipitate, utilizing Atom Probe Tomography (APT).

Furthermore, we aim to compare the modified Inconel 738LC with the typical composition, elucidating changes in interface energy and γ/γ′ misfit. Microstructure analyses will be conducted using a combination of Scanning Electron Microscopy (SEM), Electron Backscatter Diffraction (EBSD), Electron Channeling Contrast Imaging (ECCI), and High-Resolution Transmission Electron Microscopy (HRTEM). These analyses will delve into the intricate relationship between the alloy's properties and microstructure.

**Keywords:** Ni-based superalloy; Microstructure; Ni3(Al,Ti)-type precipitates (γ′), Interface energy; γ/γ′ misfit

| P-J0650 |

# Improved cryogenic tensile properties of additive manufacturing processed STS316L steel by the reusable powder

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## Abstract

Laser powder bed fusion(L-PBF) has attracted great interest in the aerospace sectors because it can produce complex parts with high accuracy. In the L-PBF of metallic materials, costs and material yields strongly depend on the ability to reuse powder efficiently. However, some of the powders are exposed to high temperatures during the manufacturing process resulting in an alteration of the feedstock properties if it reused. Therefore, to investigate the change of the powder during the process and the effect of the powder on the laminated parts, we tried to investigate the effect of reused STS316L powders on the tensile properties of their printed products under 77 K conditions. The powders were used, collected, sieved, and reused up to 15 times with all steps from the original powder.

**Keywords:** L-PBF, STS316L, cryogenic, tensile test, reusable powder

# POSTER Session 1

## Symposium K : High-Entropy Materials and Amorphous Materials

**P-K0615** **Synthesis of Single-Crystal High-Entropy Carbide-Nanocrystals with developed {100} and {111} planes and evaluation of water splitting properties**
Junmo Jeong (Chungnam National University, Korea)

**P-K0690** **Evaluation of Phase Stability of High-Entropy Alloys by First-Principles Calculations**
Kazuma Ogushi (Osaka University, Japan)

**P-K0776** **Radiation Induced Steady State Grain Boundary Structures and Their Dynamics**
Ian Chesser (Los Alamos National Laboratory, USA)

**P-K0832** **Effects of Oxidation and Crystallization on Formability of a Zr-based Metallic glass in Thermal Nanoimprint Lithography**
Sangtae Woo (Pusan National University, Korea)

**P-K0958** **Microstructural Evolution and Tensile Property Enhancement of Low-cost Fe-24Mn-22Ni-12Cr Medium-entropy Alloy by Cryogenic Caliber Rolling**
Jae-Ho Lee (Korean Institute of Materials Science(KIMS), Korea)

**P-K1122** **A feasibility study on microstructure and corrosion behaviour of Fe-based HVOF metallic glass coating layer**
Junhee Han (Korea Institute of Industrial Technology, Korea)

| P-K0615 |

# Synthesis of Single-Crystal High-Entropy Carbide-Nanocrystals with developed {100} and {111} planes and evaluation of water splitting properties

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## Abstract

The metal industry accounts for 38.3% of the greenhouse gas emissions by industry sector, and emits the most greenhouse gases in the industrial sector. In order to reduce greenhouse gas emissions, research on reducing iron ore to hydrogen is actively underway in the metal industry, and high-purity hydrogen is required for this purpose. High-purity hydrogen is mostly obtained through electrolysis, and since Pt, an expensive metal, is used as a catalyst, researches have been conducted to replace it.

In this study, Single Crystal High Entropy Carbide Nanocrystals (Ti0.2Zr0.2Hf0.2Ta0.2Nb0.2C) with exposed {100} and {111} planes were used as catalysts for hydrogen generation. We have developed a novel magnesiothermic reduction method to prepare HEC. It was confirmed that the resulting HEC inhibited the growth of {111} planes in liquid Ni and the growth of {100} planes in liquid Al. The HEC showed excellent electrocatalytic activity for the hydrogen generation reaction with a low overpotential of 0.171 V based on 10 mA/cm2.

**Keywords:** High-Entropy-Carbide, Hydrogen-Evaluation-Reaction, Catalyst,

| P-K0690 |

# Evaluation of Phase Stability of High-Entropy Alloys by First-Principles Calculations

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## Abstract

Computational material design for newly functional high-entropy alloy (HEA) using first-principles calculations is not straightforward due to the disorder and huge combinatorial freedom of the choice of constituent elements. We need a large supercell to simulate random configuration and taking configuration average becomes very difficult. To solve these difficulties, we employ the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA). The KKR-CPA provides effective way to calculate configuration average of physical properties of random alloys. In this paper, for each 5-component HEA, we calculate formation energies of 4, 3 and 2-component alloys those are composed from the elements included in the 5-component HEA. By comparing calculated formation energies with the formation energy of the 5-component HEA, we can evaluate its stability.

We apply this method to typical HEAs, such as CrMnFeCoNi and CrMnFeCoCu. In CrMnFeCoNi, we found that Cr is separated on its own in the low-temperature regime, while above 1100 K, the atomic configuration is disordered, and HEA is formed. On the other hand, in CrMnFeCoCu, the Cu is separated by itself up to 2500 K, making it difficult to become a HEA. These results reproduce the difference between these 2 kinds of 5-component alloys, and it corresponds qualitatively well with the experimental observations. The evaluation of the phase stability of HEA by this method will be useful to pick up a candidate HEA from a viewpoint of synthesizability.

**Keywords:** High-Entropy Alloys, First-Principles Calculations, Phase Stability, KKR-CPA

# Radiation Induced Steady State Grain Boundary Structures and Their Dynamics

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## Abstract

The complex radiation-induced defect evolution of alloys near grain boundaries (GBs) is still poorly understood. In this work, we employ atomistic simulations to study the high radiation dose limit of grain boundary (GB) structures for many types of GBs in FCC Ni. We find that, upon continuously loading a GB with Frenkel pairs in the athermal limit, a steady state disordered GB structure is reached with excess properties which fluctuate around a constant value. The steady state irradiation response of GBs has similarities to the dynamics of both irradiated glasses and crystals with a spectrum of glassy to crystalline behavior depending on GB type. Collective dynamics are commonly observed including string-like structural excitations and GB migration. Radiation induced steady state GB structures can typically be described as a superposition of the initial, pristine GB structure with absorbed interstitials, a non-equilibrium vacancy atmosphere and accumulated line defects such as disconnections and dislocations. Steady state GB structures vary with macroscopic GB crystallography, but are found to depend only weakly on initial metastable GB structure. The mechanical responses of pristine and irradiated GB structures are compared under an applied shear stress and are found to differ significantly in many, but not all cases. We discuss implications of this study for engineering radiation damage tolerant alloys.

**Keywords:** Grain boundaries, radiation damage, Nickel alloys, point defects, atomistic simulation

| P-K0832 |

# Effects of Oxidation and Crystallization on Formability of a Zr-based Metallic glass in Thermal Nanoimprint Lithography

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## Abstract

The transfer of nanopatterns onto material surfaces has found broad applications in various fields including bioengineering, optics, and energy harvesting. Thermal imprint lithography stands out as a cost-effective and time-efficient method; however, its use has been limitedly applied to some polymer materials.

Metallic glasses exhibit polymer-like formability above their glass transition temperature, which allows for precise patterning through thermal nanoimprint lithography despite their metallic nature. Previous studies on imprinting metallic glasses have focused on noble metal-based alloys, such as Pd or Pt, that are not prone to oxidation during the process. However, for functional utilization of nanopatterned surfaces, it is advantageous to form metal oxides, such as ZrO2 and Cu2O, on the metal surface. This requires expanding the range of alloys that can be imprinted.

In this study, we selected a Zr-based metallic glass for the imprinting process due to its wide supercooled liquid region and high thermal stability. Cross-sectional TEM analysis was performed to investigate the oxidation and crystallization behavior during the imprinting process. The effect of temperature and pressure on the crystallization and oxidation behaviour of the Zr-based metallic glass, and the main factors related to formability will be discussed.

**Keywords:** Metallic glass, Thermal Plastic Forming, Imprint Lithography, Micro/Nano pattern, Metal oxide

| P-K0958 |

# Microstructural Evolution and Tensile Property Enhancement of Low-cost Fe-24Mn-22Ni-12Cr Medium-entropy Alloy by Cryogenic Caliber Rolling

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## Abstract

High- and medium-entropy alloys (HEAs/MEAs) have been extensively developed over the last two decades owing to their superior mechanical performances from cryogenic to high temperatures. However, the high raw material costs of recently developed HEAs/MEAs limit their practical applications. In this study, we designed cost-effective Co-free, Fe-based MEAs based on thermodynamic calculations. To enhance the yield strength of the MEA, multi-pass caliber rolling, which has been recognized for improving the yield strength, was implemented at room and cryogenic temperatures. The yield strengths substantially improved from 229 MPa for the annealed specimen to 862 MPa for the sample caliber-rolled at cryogenic temperatures while maintaining good ductility. Based on the above findings, the effects of multi-pass caliber rolling at cryogenic temperatures on the microstructural evolution, mechanical properties, and deformation behavior are discussed.

Jae-Ho Lee K: High-entropy Materials and Amorphous Materials

**Keywords:** Medium-entropy alloy, Caliber-rolling, Cryogenic temperature, Microstruvture, Mechanical property

| P-K1122 |

# A feasibility study on microstructure and corrosion behaviour of Fe-based HVOF metallic glass coating layer

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## Abstract

Fe-based metallic glasses (MGs) have gained attention for their outstanding high-temperature properties and corrosion resistance, making them attractive for elevated-temperature applications. This study investigates the use of Fe-based metallic glasses as coatings for biomass boiler tubes using high-velocity oxygen fuel (HVOF) thermal spray processing.

Microstructure and thermal properties of Fe-based metallic glasses were studied through differential scanning calorimetry, monochromatic Co-Kα X-ray diffraction, and scanning electron microscopy. Corrosion behaviour was evaluated using potentiodynamic polarization curves in acidic solutions. Based on results, Fe-based MG coatings exhibited a passivation behaviour with effective anti-corrosion effects. Corrosion resistance and high temperature performance of the Fe-based HVOF MG coating were tested in biomass boiler conditions, revealing strong thermal stability and protection effects. This research highlights the potential of Fe-based metallic glasses as an anti-corrosion coating material for biomass boiler tubes.

**Keywords:** Fe-based Metallic glass, corrosion, potentiodynamic polarization, HVOF

# POSTER Session 1

## Symposium L : Composite, Coating and Hetero-Materials

**P-L0184** **Photocatalytic Characterization of Zn-TiO2/Phosphor composite Synthesized by Hydrothermal and Coprecipitation Methods**
Hye Rin Jeong (University Of Seoul, Korea)

**P-L0349** **Molecular dynamics study on viscous behaviour of water molecules on fatty acid-coated calcite nanosurface**
Shumpei Mori (Okayama University, Japan)

**P-L0535** **Functionally graded materials with high dimensional stability and near-zero thermal expansion around room temperature**
Xiaokang Zhong (Hefei Institute of Physical Science, Chinese Academy Science, China)

**P-L0949** **Effect of heat treatment on high temperature wear behavior of TiC/FC250 composites**
Yu Jin Im (Dong-Eui University Korea)

**P-L1052** **Synergy of strength-ductility in heterostructured alloys fabricated by laser-cladding**
Hyo Jeong Ha (POSTECH, Korea)

| P-L0184 |

# Photocatalytic Characterization of Zn-TiO2/Phosphor composite Synthesized by Hydrothermal and Coprecipitation Methods

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## Abstract

Zn-impregnated TiO2 nanopowders were supported on long-lasting phosphors by the chemical wet processing of hydrothermal and coprecipitation methods. The photocatalytic reactivity of the Zn-TiO2/long-lasting phosphors was evaluated as different TiO2 coating times and processes. To improve the photocatalytic efficiency the TiO2 coating times and process were varied. The fabricated Zn-TiO2/long-lasting phosphor composites were characterized using EDS and XPS for component analysis, BET for specific surface area measurement, and FE-SEM for surface morphology images. The results showed that TiO2 nanopowders were evenly coated on the long-lasting phosphor, Sr4Al14O25:Eu,Dy and the honeycomb-shaped TiO2 coating layers were observed for the fabricated Zn-TiO2/long-lasting phosphor composites, the phot-decomposition of toluene gas was investigated using GC under UV and visible light irradiation. The results showed that the photocatalytic efficiency under visible light was 33 % after 1 hour for the sample of TiO2-coated once, and 100 % decomposition efficiency was achieved after 1 hour for the sample of TiO2-coated twice by the precipitation method. When TiO2-coated twice by hydrothermal method, 100 % decomposition efficiency was achieved after just 30 minutes under visible light irradiation.

**Keywords:** TiO2, Photocatalysts, Sr4Al14O25:Eu,Dy phosphor, hydrothermal process, coprecipitation

| P-L0349 |

# Molecular dynamics study on viscous behaviour of water molecules on fatty acid-coated calcite nanosurface

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## Abstract

Nanometer-order Precipitated Calcium Carbonate (PCC) is one of the nanomaterials used as filler materials, drug, and so on. It has been reported that when surface-treated PCC with fatty acids is blended with adhesives, the viscosity increases more effectively than that of non-treated PCC, providing excellent rheological properties. However, the mechanism of it is not yet well understood. In addition, the surface treatment makes the particles hydrophobic, which reduces the amount of water adsorbed by calcite. Such hydrophobicity of the nanoparticles is important for the stability in its use of sealants.

Using molecular-dynamics simulations, we investigated the viscous behaviour and hydrated state of water molecules on calcite with stearic acid coating. We have previously performed first-principles MD simulations to investigate the structure of fatty acid molecules adsorbed on a calcite surface and found that the most stable adsorption state is achieved when the hydrophilic group of the stearic acid molecule forms a bond with the calcium atom on the calcite (104) surface.[1] Here we show the presence of surfactants surrounded by water molecules on calcite is expected to increase the viscosity. The details of these analyses along with search for stable hydrated state of surface-active agents will be discussed in the presentation.[1] N. Machida, M. Misawa, Y. Kezuka, and K. Tsuruta, "First-principles Analysis of Stearic Acid Adsorption on Calcite (104) Surface,",e-JSSNT 20, 261 (2022).

**Keyword:** nanomaterials, calcium carbonate, surface coating, viscosity, molecular dynamics

| P-L0535 |

# Functionally graded materials with high dimensional stability and near-zero thermal expansion around room temperature

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## Abstract

In order to meet the requirements of thermal stability of precision instruments and microelectronic devices, Cu2P2O7/Al-Si functionally graded materials were prepared by pressure infiltration. The results show that not only the strong bonding between Cu2P2O7 and Al-Si alloy is achieved, but more importantly, the gradient microstructure is introduced into the materials. The gradient microstructure is characterized by the grain-size gradient of the Al-Si alloy, which leads to the gradient change of the thermal expansion coefficient along the thickness direction of the materials. The materials show high dimensional stability and near-zero thermal expansion around room temperature when the thickness of the Al-Si alloy part is 20 μm, which result in ideal materials for precision instruments and microelectronic devices.

**Keywords:** Functionally graded materials; Gradient microstructure; Dimensional stability; Near-zero thermal expansion

| P-L0949 |

# Effect of heat treatment on high temperature wear behavior of TiC/FC250 composites

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## Abstract

In this study, TiC reinforced FC250 matrix composites were fabricated by a liquid pressing infiltration process. Heat treatment was performed to improve the mechanical properties, and a high temperature wear test was conducted to confirm the wear behavior of the composite.

**Keywords:** behavior, metal matrix composites, TiC reinforcement, heat treatment, microstructure.

| P-L1052 |

# Synergy of strength-ductility in heterostructured alloys fabricated by laser-cladding

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## Abstract

To ensure the stability of the constituent products for industrial applications, a superior combination of strength and ductility is required in materials. In this study, we propose a simple process to develop heterostructured alloys by laser-cladding a thin layer on the surface of the wrought 316L stainless steels. The enhanced twining activity localized in the coating region generated high mechanical incompatibility. Furthermore, the HDI (hetero deformation induced) strengthening of heterostructured samples resulted in an enhanced strength – ductility synergy. The laser clad wrought samples exhibited enhanced strength and ductility compared to homostructured sample. This study presents a new direction for the use of laser-cladding to produce a heterostructurally-designed alloy with superior strength-ductility synergy.

**Keywords:** Heterostructures; Laser-cladding; Stainless steel; Laser deposition;

# POSTER Session 1

## Symposium M : Nano Materials and Nano Severe Plastic Deformation

**P-M0094** **Enhanced Stability in Strain Sensors with Pore-Free Encapsulation and Deep Learning-Based Human Motion Recognition**
HyunSik Shin (Sungkyunkwan University, Korea)

**P-M0120** **Self-Healing Wearable Flexible Heaters Based on MXene/Polycaprolactone Composites and Silver Nanowire Electrodes**
Su Bin Choi (Sungkyunkwan University, Korea)

**P-M0634** **Formation of metastable phase in Si1-xGex crystals by severe plastic deformation under high pressure**
Marina Takaira (Kyushu University, Japan)

**P-M0918** **Influence of deformation degree by High-Pressure Torsion on Ti-25at%Nb alloys synthesized from elemental powders.**
Kathy Gonzalez (Instituto Tecnológico De Costa Rica, Costa Rica)

**P-M0998** **Enhancement of coercivity for microfabricated Sm(Fe-Co) dot arrays with Sm seed layer**
Shintaro Hatanaka (Tohoku Gakuin University, Japan)

**P-M1067** **Nanomechanical behavior of ultrafine-grained structural alloys processed by high-pressure torsion technique**
In-Chul Choi (Kumoh National Institute of Technology, Korea)

| P-M0094 |

# Enhanced Stability in Strain Sensors with Pore-Free Encapsulation and Deep Learning-Based Human Motion Recognition

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## Abstract

Flexible strain sensors have gained significant interest in various fields, including electronic skin (E-skin), human-machine interfaces, and soft robotics. The long-term use of these sensors often results in damage or cracks in the electrodes, prompting researchers to explore self-healing mechanisms to address this issue. However, traditional self-healing functions often fail to fully restore the original mechanical properties of the sensors. To overcome this limitation, our study combines self-healing polymers with electrospinning techniques to fabricate encapsulated sensors. Unlike conventional encapsulation methods such as lamination or spin coating, which tend to produce pores that can degrade the electrode's performance, we employ a pore-free encapsulation approach. Our fabricated sensors demonstrated excellent mechanical properties, exhibiting only a 25% increase in resistance after 5,000 stretching tests at 30% strain, and negligible resistance changes after 5,000 bending tests with a curvature radius of 300 μm. We tested the encapsulated sensors in wearable applications by attaching them to various joints, such as elbows, wrists, fingers, and knees, and collected a total of 4,500 electrical signals from a range of motion tests. Notably, the electrical signals generated by different joint movements displayed distinct graph behaviors and figures. To analyze these signals, we designed a deep learning model that combines a Convolutional Neural Network (CNN) optimized for image classification with a Long Short-Term Memory (LSTM) network optimized for time series data classification. After pre-processing the collected data, we applied it to our deep learning model, which successfully classified joint motion movements with a high accuracy of 95.13%. This study demonstrates the potential of combining self-healing polymers, electrospinning techniques, and advanced deep learning models for the development of robust and reliable flexible strain sensors for a variety of applications.

**Keywords:** Encapsulation, Pore-free sensors, Flexible, Self-healing, Deep learning

| P-M0120 |

# Self-Healing Wearable Flexible Heaters Based on MXene/ Polycaprolactone Composites and Silver Nanowire Electrodes

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## Abstract

Flexible heaters have attracted considerable attention in recent years due to their promising applications in wearable devices, such as therapeutic patches and heated garments, which significantly enhance the user experience and functionality. For these heaters to be successfully integrated into long-lasting wearable systems, they must possess self-healing properties that allow them to recover from damage incurred during use. Although numerous studies have investigated the development of self-healing electronic devices, many of these solutions rely on external energy sources, such as heat or light, to activate their self-healing mechanisms. In this study, we report on the fabrication of a novel spontaneous self-healing heater (SHH) that does not require additional external processes, unrelated to the device's primary operation, for self-healing to occur. Our SHH was engineered using electrospun polycaprolactone (PCL) fibers, which possess a relatively low melting point of 60 °C. As an electrode layer, Ti3C2TX MXene nanosheets and silver nanowires (AgNW) were coated onto the surface of the PCL fibers. PCL, on its own, is generally unsuitable for heater applications due to its low melting point. However, the incorporation of MXene nanosheets as a structural stabilizer enabled the fabrication of an MXene/PCL composite that exhibited both thermal stability at elevated temperatures and self-healing capabilities at lower temperatures. The AgNW-coated MXene/PCL fibers exhibited outstanding electrical conductivity and displayed temperature increases in proportion to the applied voltage, thereby validating their utility as heater elements. To assess the self-healing properties of the SHH, we manually introduced cracks onto the heater surface. When a voltage of 1.5 - 1.6 V was applied, the temperature of the SHH increased to beyond 60 °C, surpassing the melting point of PCL. This temperature elevation facilitated the complete healing of the cracks without the need for any additional external processes. The results of our study indicate that SHHs can autonomously repair damage sustained during everyday use of wearable heaters, eliminating the necessity for external interventions to enable self-healing. This innovative approach to designing flexible heaters holds significant potential for the development of durable and self-sufficient wearable systems.

**Keywords:** Heater, Self-healing, MXene, Silver nanowire, Fiber

| P-M0634 |

# Formation of metastable phase in Si1−xGex crystals by severe plastic deformation under high pressure

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## Abstract

Si1−xGex crystals are an environmentally and human-friendly material and are expected to be applied to thermoelectric conversion devices and infrared lenses. Since Si1−xGex is an all-proportional solid solution, the lattice constant and band gap of Si1−xGex crystals can be varied continuously by Ge concentration (x). Furthermore, if metastable phases can be utilized, Si1−xGex crystals with various band gaps ranging from semimetals to semiconductors can expected to be developed. Previously, we have applied high-pressure torsion (HPT) to Si0.5Ge0.5 at a nominal pressure of 24 GPa and found that a body-centered-cubic (bc8) structure was formed as a metastable phase. However, the metastable phases of SiGe having a different x are unknown. In this study, we applied HPT to Si1−xGex crystals at a nominal pressure of 24 GPa. The HPT-processed samples without anvil rotation (N = 0) consisted of diamond-cubic (dc) SiGe, while a bc8 phase appeared up to x = 0.8 when N was increased to 10. The resistivity of the HPT-processed SiGe samples after N = 0 increased for $x \leq 0.5$ but decreased for $x \geq 0.7$, and then decreased or slightly increased as N increased to 10 despite grain refinement for all x cases. These results indicate that bc8-Si1−xGex shows semimetallic properties.

**Keywords:** severe plastic deformation, high-pressure torsion, SiGe, metastable phase

| P-M0918 |

# Influence of deformation degree by High-Pressure Torsion on Ti-25at%Nb alloys synthesized from elemental powders.

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## Abstract

Beta Titanium alloys show potential application for medical implants due to their lower elastic modulus compared to α or α+β alloys. In this research, a Ti-25at%Nb alloy was synthesized using high-pressure torsion (HPT) from the elemental powders and subjecting the samples to a pressure of 6 GPa for 30, 50, and 100 revolutions at 1 rpm. The effect of deformation degree on the microstructure was examined, focusing on grain refinement and the formation of the β-phase during the evolution of the microstructure. Scanning electron microscopy (SEM) analysis revealed enhanced homogeneity with the equivalent strain, while X-ray diffraction (XRD) profiles exhibited an increasing prominence of signals corresponding to the β-Ti phase. Correlation of Vickers microhardness and the electrochemical behavior with grain size observations by transmission electron microscopy (TEM), it was observed that microhardness and corrosion resistance increased proportionally to the equivalent strain imposed by the HPT process. Moreover, the microhardness reached saturation when the microstructure achieved a more homogeneous distribution of nanostructured β-phase grains.

**Keywords:** beta titanium-niobium, high-pressure torsion, microstructure evolution, biocorrosion, biomedical alloys.

| P-M0998 |

# Enhancement of coercivity for microfabricated Sm(Fe-Co) dot arrays with Sm seed layer

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## Abstract

RFe12 compounds with ThMn12-type structure have been considered as promising candidates for next generation permanent magnet materials because of their excellent saturation magnetization and anisotropy field with a minimum usage of rare earth elements. Recently, we reported that the formation of anisotropic columnar structure and the achievement of large coercivity μ0Hc of 1.20 T by the addition of B to Sm(Fe0.8Co0.2)12 thin film. However, it was predicted that not only B dope but also suppression of soft magnetic phase existing between V under layer and Sm(Fe0.8Co0.2)12 layer and microfabrication play important role to achieve a high μ0Hc. In this study, in order to increase the coercivity of Sm(Fe0.8Co0.2)12 thin films, the sample with Sm seed layer was microfabricated and crystal structure and magnetic properties have been investigated. Sm/ Sm(Fe0.8Co0.2)12 thin film were prepared using an ultra-high vacuum magnetron sputtering system. Micro-fabrication of Sm/ Sm(Fe0.8Co0.2)12-B thin films was performed by electron beam lithography and Ar ion etching system. The square dot arrays showing distinct shape with a pitch width of approximately 120 nm was confirmed by SEM. The average height of the trench after etching was obtained to be 107 nm by AFM. It was confirmed that Mr/ Ms was increased from 13.2 % to 21.1 % by microfabrication, but μ0Hc was slightly decreased from 0.09 T to 0.07 T.

**Keywords:** α-Fe phase, coercivity, electron-beam lithography, thin film, ThMn12-type structure

| P-M1067 |

# Nanomechanical behavior of ultrafine-grained structural alloys processed by high-pressure torsion technique

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**Abstract**

One of the best known methods to achieve grain refinement to improve the strength and ductility of structural alloys is the severe plastic deformation (SPD) process such as ECAP (Equal-Channel Angular Pressing) and HPT (High-Pressure Torsion). Among the available SPD technologies, HPT processing may be more attractive than ECAP due to a number of advantages. That is, it is a simpler technique without undesirable cracking due to high hydrostatic pressure, and can impose higher plastic strains. Extensive studies have been conducted to elucidate the changes in microstructure and hardness of structural alloys such as zinc-aluminum alloys or magnesium alloys during HPT processing at room temperature. In this study, to monitor changes in plastic deformation or dynamic mechanical properties after HPT processing two different tests were performed. First, strain-rate sensitivity and activation volume, which are useful quantitative indicators of thermally activated plastic deformation, were estimated through nanoindentation. Second, the evolution of high-cycle fatigue behavior was investigated using a small-scale bending test system at the disc edge. In both results, the changes in strain rate sensitivity, activation volume and high cycle fatigue life are discussed in terms of microstructural evolution and underlying mechanisms.

**Keywords:** High-pressure torsion, Ultrafine-grained structural alloy, Nanomechanical behavior, Nanoindentation, Small-scale bending test

# POSTER Session 1

## Symposium N : Computational Materials and Artificial Intelligence

**P-N0043** **Prediction of Flaw Detection Results and Evaluation of crucial Process Factors for Continuous Casting billet of Pipeline Steel Based on the Decision Tree Algorithm**
Fuyue Wang (Ansteel Iron & Steel Research Intitute, China)

**P-N0136** **Modelling of Hydrogen Diffusion Influenced Screw Dislocation Motion in BCC Iron**
JIAQIN XU (OSAKA UNIVERSITY, Japan)

**P-N0213** **Large-scale phase-field computation for predicting material microstructures from shape forming to sintering**
Aoi Nakazawa (Kyoto Institute of Technology, Japan)

**P-N0234** **Temperature dependent elastic properties of Mo-Ti BCC solid solutions by first principles calculation**
Junfeng Du (Tohoku University, Japan)

**P-N0278** **Investigation of a system to predict 3D microstructures from 2D cross-sectional images through machine learning and phase-field simulations**
Sota Fujikawa (Kyoto Institute of Technology, Japan)

**P-N0528** **Cluster Formation Behavior by Monte Carlo Simulation in Al-Mg-Si Alloys**
JiWook Park (Korea Institute of Industrial Technology, Korea)

**P-N0723** **Balancing Tensile Strength and Elongation in Co-reduced Martensitic Steels: A Machine Learning Approach**
SooBeen KIM (Kookmin University, Korea)

**P-N0733** **Advanced Precipitate and Dislocation Segmentation in STEM Images using U-net Architecture and Focused Region Training**
JUNYU CHOI (Kookmin University, Korea)

**P-N0834** **Prediction and mechanism explain of martensite start temperature of alloy steel via explainable artificial intelligence**
Seungbae Son (Jeonbuk National University, Korea)

**P-N0925** **XAI-aided carbon diffusivity prediction and mechanism analysis in austenite**
Seok-Jae Lee (Jeonbuk National University, Korea)

| P-N0043 |

# Prediction of Flaw Detection Results and Evaluation of crucial Process Factors for Continuous Casting billet of Pipeline Steel Based on the Decision Tree Algorithm

**Fuyue Wang**[1], Yi Ren[1*], Yongjiu Tian[2], Shuai Zhang, Shuang Wang[1], Hong Gao[1], Zherui Zhang[1]

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## Abstract

This study aimed at the need for ultra-clean pipeline steel products. The production data of pipeline steel billet was collected and used in an iron and steel enterprise, combined with the principle of metallurgy and Pearson correlation coefficient selection of crucial process characteristics of casting properties, for inspection results of pipeline steel plate as the label, the decision tree algorithm is adopted to establish the quality prediction model of pipeline steel continuous casting billet. After adjusting the model's structural parameters and model evaluation, the model with good prediction effect (AUC value of the test Set is 0.848) and good generalization ability (ΔAUC value is 0.042) was obtained. The decision tree prediction model generated in this study provides a simple, efficient, and intense interpretation of the results of the prediction method. The key points and thresholds of the process were accurately located according to the importance score (continuous casting speed ≤0.87m/min, casting superheat ≥25.5°C, RH refining time ≥11.5min). It provides help for intelligent adjustment of enterprise processes and intelligent management of product quality.

**Key words:** Decision Tree Algorithm; Continuous Casting billet; Flaw Detection; prediction model

| P-N0136 |

# Modeling of Hydrogen Diffusion Influenced Screw Dislocation Motion in BCC Iron

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## Abstract

Humanity is suffering from hydrogen embrittlement. However, a widely accepted theory of hydrogen embrittlement is still lacking. To understand the mechanism of hydrogen embrittlement, it is essential to comprehend the underlying hydrogen-defect interactions that cause embrittlement. Nevertheless, dynamics of dislocation motion influenced by hydrogen in metals is not well understood. Here, we present a model to describe a coupled dynamics between hydrogen diffusion and screw dislocation motion in BCC iron as the function of applied stress, temperature and hydrogen concentration based on an advanced Fe-H neural network potential to solve the question whether hydrogen atoms accelerate or deaccelerate screw dislocation motion. The computation results of the model suggest that hydrogen atoms instead of restricting screw dislocation, accelerate dislocation motion by reducing activation barrier of dislocation glide. Moreover, obtained hydrogen diffusion kinetics and dislocation motion are confirmed by molecular dynamics simulation. The model is expected to provide more detailed information for hydrogen embrittlement investigation.

**Keywords:** Dislocation motion; Hydrogen diffusion; Iron; Numerical simulation; Molecular dynamics

| P-N0213 |

# Large-scale phase-field computation for predicting material microstructures from shape forming to sintering

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## Abstract

Solid-state sintering is one of the most important material-processing techniques for manufacturing metal and ceramic products. Since the properties of sintered products are significantly affected by their microstructures, predicting and controlling the microstructures formed during sintering is essential for manufacturing high-performance sintered products. However, visualizing the evolution of material microstructure directly during sintering is challenging; therefore, numerical simulation studies are crucial. The phase-field method is the most effective computational method for investigating the evolution of the material microstructure and consequently preferred for simulating sintering. However, three-dimensional phase-field simulations of realistic sintering processes with sufficient particles have not yet been performed primarily due to their high computational cost.

In this study, we developed a high-performance phase-field computational method to accurately simulate the evolution of the microstructure of materials from powdered green body formation to sintering. During the powder green body formation process, massive number of grains were loaded into a mold and compressed. Subsequently, the formed green body was sintered. These series of processes were simulated on a large scale using the phase-field method.

This presentation is based on results obtained from a project, JPNP22005, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

**Keywords:** Phase-field simulation; High-performance computing; Solid-state sintering; Material microstructure

| P-N0234 |

# Temperature dependent elastic properties of Mo-Ti BCC solid solutions by first principles calculation

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## Abstract

Mo-Ti binary BCC solid solution (BCCss) is the key phase in ultra-high-temperature MoSiBTiC alloys: the room-temperature fracture toughness and ultrahigh-temperature tensile creep properties of the alloy are greatly affected by the properties of the Mo-Ti BCCss phase. The study on the temperature-dependent elastic stiffness coefficients of the Mo-Ti BCCss phase is of great significance for understanding and predicting their mechanical strength, stability and phase transition of the MoSiBTiC alloys. In this study, the atomic arrangement of a supercell was constructed by the Special Quasi-random Structure (SQS) method, and the high-temperature physical properties of Mo-Ti binary BCCss phases were evaluated by density functional theory (DFT) calculations combined with Quasi-harmonic Approximation (QHA). The influence of temperature on the elastic properties of Mo-Ti BCCss phases was analysed in terms of the bulk modulus and shear modulus, Young's modulus and Poisson's ratio. The variation of ductility of Mo-Ti BCCss phases with temperature was evaluated based on the Pugh's ratio. The results of this study can provide a useful reference for the design of Mo-Ti BCCss phase.

**Keywords:** Molybdenum, Titanium, Elastic stiffness coefficients, Quasi-random structure, First principles calculation.

| P-N0278 |

# Investigation of a system to predict 3D microstructures from 2D cross-sectional images through machine learning and phase-field simulations

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## Abstract

Considering that the microstructure of a material determines its properties, it is essential to evaluate and control it. Although microstructures of materials are typically observed two-dimensionally from their surfaces, material properties strongly depend on their 3D microstructures. Currently, 3D microstructures are observed through X-ray computed tomography or serial sectioning. However, these methods are both time and cost intensive, and systematic evaluations using these methods are not straightforward.

Machine learning is applied in various fields, including image analysis. Methods for predicting 3D microstructures through machine learning based on 2D cross-sectional images are being developed [Comput. Methods Appl. Mech. Eng., 390 (2022) 114532]. However, the insufficiency of 3D microstructural information to be learned is a critical drawback.

The phase-field (PF) method is a promising simulation method that can reproduce the material microstructures with the highest accuracy. Because the PF method can reproduce various and large numbers of 3D microstructures with improved computer performance, the results of PF simulations can be used as training data for machine learning to further improve the prediction accuracy.
In this study, we aimed to construct a machine learning system to predict 3D microstructures from 2D cross-sectional images using the results of PF simulations as training data. The accuracy of the method was confirmed by comparing the predicted 3D microstructures with the PF results.

**Keywords:** Phase-field simulation; Machine learning; Microstructure; 3D reconstruction

| P-N0528 |

# Cluster Formation Behavior by Monte Carlo Simulation in Al-Mg-Si Alloys

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## Abstract

The applications of Al-Mg-Si alloys are continuously expanding beyond automotive, marine, and construction industries. There is a demand for alloys with even more superior properties. Al-Mg-Si alloys are known to obtain excellent mechanical properties through precipitation strengthening via heat treatment. In this point of view, the formation of clusters plays an important role in precipitation behavior. Numerous research studies have been conducted using various tools for precise analysis, such as transmission electron microscope (TEM), scanning electron microscope (SEM), X-ray diffraction (XRD), three dimensional atom probe (3DAP), and computer simulation. Computer simulation is particularly beneficial in reducing costs and saving time among these tools. Monte Carlo simulation is one of the simulation methods utilized by many research groups to investigate cluster analysis in alloys. In this study, we employed Monte Carlo simulation to predict the cluster formation behavior of Al-Mg-Si alloys. Furthermore, we analyzed the tendencies based on the results of the number, size, and composition of the formed clusters.

**Keywords:** Al-Mg-Si Alloy, Monte Carlo Simulation, Cluster Analysis, Precipitation, Computer Simulation

| P-N0723 |

# Balancing Tensile Strength and Elongation in Co-reduced Martensitic Steels: A Machine Learning Approach

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## Abstract

Secondary hardening martensitic steels are advanced structural materials that demonstrate a remarkable balance between strength and toughness. These outstanding mechanical properties are primarily attributed to the precipitation of secondary M2C carbide during the aging heat treatment. In particular, the refinement of nanosized M2C is crucial to achieving 2 GPa-grade tensile strength without degrading elongation, but this typically requires significant amounts of costly alloying elements, such as Co and Ni. Consequently, altering the alloy to reduce Co and Ni content presents a substantial challenge for the wider adoption of these materials across various industries. In our previous research, we found that the addition of V can effectively counteract the mechanical property deterioration in Co-reduced alloy steels. However, increasing V content may result in the introduction of a substantial amount of primary carbides into the alloy matrix, which complicates the promotion of effective secondary hardening during the aging treatment. Although this challenge can be addressed by raising the austenitizing temperature, this strategy is constrained by the risk of coarsening the prior austenite grain size (PAGS), potentially leading to intergranular fracture and a subsequent decrease in elongation. Therefore, identifying optimized process conditions that can both maximize the decomposition of primary carbides and minimize PAGS—thereby achieving a balance in trade-off properties (tensile strength vs. elongation)—is essential. In this study, we propose a methodology that combines active learning with an objective function derived from various linear and non-linear regression models. This approach allows for the optimization of processing conditions without needing to physically test tensile specimens.

**Keywords:** Secondary hardening, Active learning, Process optimization, Trade-off properties, High Co-Ni martensitic steels

| P-N0733 |

# Advanced Precipitate and Dislocation Segmentation in STEM Images using U-net Architecture and Focused Region Training

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## Abstract

Recently, the U-net architecture, based on fully convolutional networks (FCNs), has gained significant attention for its exceptional performance in image segmentation. Particularly in the field of image analysis, this architecture has proven to be highly effective in generating accurate results. In this study, we employ the U-net architecture to segment precipitates and the matrix in Scanning Transmission Electron Microscopy (STEM) images and detect dislocations around the interface. To achieve this, we propose a novel system called the "Segregation and Merging system." In the segregation step, we convert the input image data into two distinct types of data. The first type is used for segmenting dislocations, while the background includes both precipitates and the matrix. To capture and learn localized features, such as dislocations, more effectively, we introduce a concept called "Focused Region Training." The second type of data is used to segment precipitates and the matrix, employing separate models for each type, resulting in unique outputs. In the merging step, we combine the outputs from both models to generate a multi-label segmentation map. This approach effectively addresses common challenges related to low accuracy and overfitting, commonly associated with limited computational power and image resolution. Notably, our method significantly improves upon existing techniques. Furthermore, we explore potential applications of our findings, such as measuring distances between dislocations. Leveraging the multi-label segmentation map, we extract valuable information that aids in the further analysis and characterization of materials. Overall, our study presents a novel method for image segmentation using the U-net architecture.

**Keywords:** U-net architecture, image segmentation, STEM image, dislocation, Segregation and Merging system, focused region training

| P-N0834 |

# Prediction and mechanism explain of martensite start temperature of alloy steel via explainable artificial intelligence

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## Abstract

This study proposes a machine learning model to predict the martensite start temperature (Ms) of alloy steels. We collected 219 usable data from the literature, and Adjusted the hyperparameters to propose an accurate machine-learning model. Artificial neural networks (ANN) exhibited the best performance compared with existing empirical equation. The prediction mechanisms and feature importance of the ANN with regards to the whole system were discussed via the Shapley additive explanation (SHAP).

**Keywords:** Machine learning(ML), Martensite start temperature, Explainable artificial intelligence(XAI), Prediction mechanism

| P-N0925 |

# XAI-aided carbon diffusivity prediction and mechanism analysis in austenite

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## Abstract

Carbon diffusivity in austenite is an important feature for controlling the overall properties of steels during heat treatment, such as annealing and normalizing. However, accurately predicting carbon diffusivity and analysing its features remain challenging tasks in model improvement. In this study, machine learning methods were employed to precisely predict carbon diffusivity and provide detailed insights into the prediction mechanisms of its features. Shapley additive explanation (SHAP) method was utilized to analyse the feature mechanisms. From the literature, 263 usable datasets were collected, and then analysed and three outliers were excluded. Hyperparameters are searched using five-fold cross-validation and a grid search. Random forest regression (RFR) was selected based on the determination coefficient. The RFR is compared with an empirical equation using training, testing, and additional datasets. The importance and mechanisms of input features such as temperature, carbon concentration, Cr, Ni, Si, Al, Mn, and Mo were discussed based on the calculation results of the Shapley value. Temperature exhibited the most significant influence on carbon diffusivity, followed by carbon concentration, Cr, Si, Mo, Ni, Al, and Mn. While temperature, carbon concentration, Mo, Ni, and Mn increased carbon diffusivity, Cr, Si, and Al decreased carbon diffusivity.

**Keywords:** Carbon diffusivity; Explainable artificial intelligence(XAI); Machine learning; Shapley additive explanations(SHAP); Prediction mechanism

# POSTER Session 1

## Symposium O : Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**P-O0329** **Deoxidation of Ti-6Al-4V alloy melt using hydrogen plasma arc melting**
Yuya Matsuzaki (Tohoku University, Japan)

**P-O0604** **Improvement of Lithium-Ion Battery Anode Performance Using Mg Base Alloy Electrode**
Chaeyeon Yeom (Chungnam National University, Korea)

**P-O0731** **Influence of Annealing Conditions on the Microstructure and Magnetic Properties of Nd-Fe-B Sintered Magnets**
Gian Song (Kongju National University, Korea)

**P-O0741** **Extraction behavior of rare earths elements in hydrogen treated permanent magnets**
Sangmin Park (Korea Institute of Industrial Technology, Korea)

| P-O0329 |

# Deoxidation of Ti-6Al-4V alloy melt using hydrogen plasma arc melting

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## Abstract

Ti-6Al-4V is a common Ti alloy because of its superior heat treatability and balance of strength and ductility. To expand its applications further, its production cost is required to be lowered using off-grade Ti sponges and its scraps as raw materials for melting. Deoxidation of Ti melt is crucial in establishing a reasonable production process as oxygen is a main impurity in Ti owing to its high chemical affinity with Ti. We developed a deoxidation process for commercially pure Ti melts using two-step plasma arc melting under Ar-H2 and Ar atmospheres [1]. We applied this process to Ti-6Al-4V and investigated its effect on hydrogen and oxygen contents in the melts.

Ti-6Al-4V alloys with initial oxygen contents of 0.141, 0.276, and 1.43 mass% were used as raw materials and subjected to the two-step plasma arc melting. In addition, one-step melting varying the hydrogen partial pressure was performed. Thereafter, hydrogen and oxygen contents in the melts were analyzed in the depth and surface directions of the ingot.

Following the two-step plasma arc melting under the optimal condition, the oxygen contents at the surface of the alloy melts reduced from 0.141, 0.276, and 1.43 mass% to 0.100, 0.163, and 0.989 mass%, respectively. After the one-step melting, the oxygen contents decreased to 0.116, 0.227, and 1.13 mass%, respectively. The hydrogen content in the melt increased with increasing hydrogen partial pressure.

[1] M. Watanabe et al.: Metall. Mater. Trans. B, 50 (2019) 1553–1558.

**Keywords:** refining, melting, oxygen, Ti alloy, recycle

| P-O0604 |

# Improvement of Lithium-Ion Battery Anode Performance Using Mg Base Alloy Electrode

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## Abstract

For lithium-sulfur (Li-S) or high-nickel content NCM cathodes, which are intended for electric vehicle drive, the theoretical capacity of the cathode is around 300-1,000 mAh/g However, when using graphite as the anode material with a theoretical capacity of approximately 300mAh/g . the performance of secondary batteries can be constrained due to limitations of the graphite material. As a result, current research is focused on lithium metal electrodes with high capacity and low reduction potential. However, the formation of lithium dendrites during repetitive charge-discharge cycles poses a significant obstacle to the commercialization of lithium metal electrodes. Various electrode materials are being studied as alternatives to suppress dendritic growth, and magnesium (Mg) is one such material. Mg has a theoretical capacity of 2150 mAh/g, and Mg-Li alloy not only has high lithium ion diffusion coefficient but also exhibits a large lithium solubility, unlike other alloy system. It forms a solid solution when lithium is plated, thereby inhibiting the growth of lithium dendrites. However, when pure Mg is used as the electrode material, the formation of a high surface resistance layer during charge-discharge cycles becomes an issue leading to a decrease in long-term cycle stability.

This study explores the application of a Mg alloy electrode and investigates the potential of enhancing charge-dischage characterisitics by controlling particle size. Smaller particles can suppress the formation of the surface resistance layer addressing the issue with Mg electrode material, while increasing surface area for improved long-term cycle stability and capacity.

**Keywords:** Mg base anode, lithium-ion battery, anode material,

| P-O0731 |

# Influence of Annealing Conditions on the Microstructure and Magnetic Properties of Nd-Fe-B Sintered Magnets

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## Abstract

Sintered Nd-Fe-B magnets are representative magnetic materials that exhibit superior performance, more than 10 times better than other magnetic materials, making them widely utilized in various industrial fields since the fourth industrial revolution, including electric vehicle motors, robot actuators, and generator modules. Typically manufactured through sintering processes, recent studies have reported numerous research efforts focused on enhancing the magnetic properties by controlling the microstructure through various processing techniques. In particular, it has been reported that significant improvement in coercivity can be achieved by controlling the distribution and morphology of the Nd-rich phase formed at the grain boundaries through post-sintering heat treatment, thereby suppressing magnetic interactions near grain boundaries.

In this study, the influence of microstructure on the magnetic properties of Nd-Fe-B magnets manufactured through sintering processes at various heat treatment temperatures was investigated. Alloy powders with fine Nd2Fe14B grains were produced through strip casting and jet milling, followed by sintering. The sintered samples underwent a secondary heat treatment at three different temperatures: 460°C, 500°C, and 540°C, following the primary heat treatment at 850°C. SEM, EBSD, and TEM analysis were conducted to analyze the changes in the morphology, distribution, and fraction of the Nd-rich phase formed at the grain boundaries corresponding to each heat treatment temperature, in order to understand the impact of these microstructural variations on the magnetic properties of Nd-Fe-B magnets.

**Keywords:** Nd-Fe-B sintered Magnet, Magnetic Properties, Coercivity, Nd-rich phase, Annealing processes

**Acknowledgements**

This work was supported by Korea Evaluation Institute of Industrial Technology (KEIT) grant funded by the Korea government (MOTIE) (Project No. 20010817, Technology for the ecofriendly rare earth refining grom used motors and manufacture of permanent magnet materials)

| P-O0741 |

# Extraction behavior of rare earths elements in hydrogen treated permanent magnets

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## Abstract

Rare earth permanent magnets are experiencing a significant increase in demand as a key power material within the green mobility sector due to rapid industrial development. However, rare earth (RE) resources are limited to specific countries, causing a global supply imbalance. As a result, research on rare earth recycling for resource sustainability is being continuously conducted. The liquid metal extraction method is one promising technique for the recycling of rare earth resources, as it enables the environmentally friendly recovery of rare earths in metallic form based on the selective reactivity between solvent metal Mg and rare earths in permanent magnets, without the need for separate reduction processes. However, the formation of RE-Fe intermetallic compounds and rare earth oxides during extraction leads to low extraction efficiency, necessitating research on phase control to enhance the reactivity between Mg and rare earths.

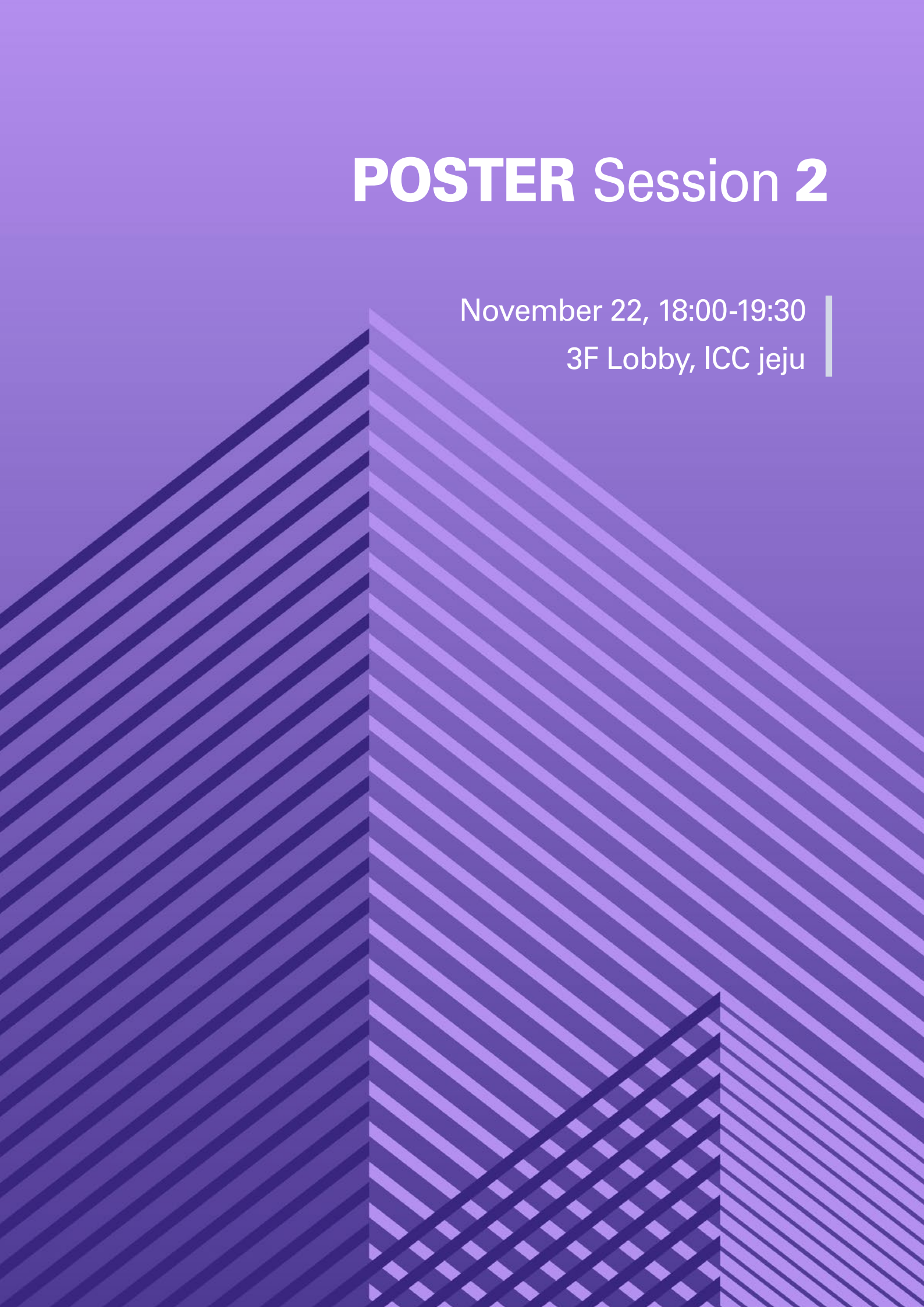
Therefore, in this study, pre-treatment utilizing hydrogen, which exhibits high reactivity with rare earths, was conducted to control factors inhibiting rare earth extraction, and liquid metal extraction research was performed. The hydrogen treated powder under the established optimal conditions was utilized for liquid metal extraction, and the extraction behavior of rare earths was confirmed through observation of phase transformations. Ultimately, by employing hydrogen pre-treatment, the inhibiting factors for rare earth extraction were suppressed, and an extraction efficiency of over 99% was achieved.

**Keywords:** Rare earths elements, Permanent magnet, Recycling, Liquid metal extraction, Hydrogen pre-treatment

# **POSTER** Session **2**

November 22, 18:00-19:30

3F Lobby, ICC jeju



# POSTER Session 2

## Symposium A : Advanced Steels and Properties

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Toya Hada (National Institute of Technology (KOSEN), Korea)

**P-A0070** **Microstructure control and stenghtening-toughening mechanism of 68.4Gpa·% grade cold rolled steel**
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**P-A0082** **Effect of carbide coarsening behaviour on tensile properties of Cr alloying medium-Mn steel**
Shengrui Su (University of Science and Technology Beijing, China)

**P-A0084** **Heterogeneous ultrafine/fine-grained austenitic stainless steel: high strength and ductility**
Shuyi Quan (University of Science and Technology Beijing, China)

**P-A0098** **Corrosion Behaviors of U75vh, R350lht Heavy rail in Simulated atmosphere**
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Jin-young Kim (Hanyang University, Korea)

**P-A0203** **Effect of Microstructure on Mechanical Anisotropy of API X70 Linepipe Steels for Electrical Resistance Welding**
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**P-A0205** **Effect of Nb, Ti, and V additions on Hydrogen Embrittlement of Tempered Martensitic Low Alloy Steels**
Hee-Chang Shin (Seoul National University of Science and Technology, Korea)

**P-A0231** **Development of 800MPa Grade Hot-Rolled High Strength Ferrite Steel with Excellent Ductility and Low Yield Ratio**
Yajun Hui (Technology Institute of Shougang Group Co., Ltd., China)

# POSTER Session 2

**P-A0295** **Effect of center segregation on low temperature impact toughness of welding heat-affected zone of pipeline steel**
Fujian Guo (Yangjiang Advanced Alloys Laboratory, China)

**P-A0313** **Improvement of Impact Properties at Low Temperatures for 0.13C Cast Steel**
Yusuke Ochi (Hiroshima University, Japan)

**P-A0325** **A Study on the Improvement of Low Temperature Impact Toughness and Microstructure Changes of ERW X70 Steel Pipe**
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**P-A0703** **Analysis of Phosphating Defects for Hot-dip Zn-Al-Mg coated Steels**
Ning Cai (Shougang Group Research Institute of Technology, China)

**P-A1070** **Effect of core-shell type second phase formed by interrupted-quenching and intercritical-annealing on mechanical property in a medium manganese steel**
Toshihiro Tsuchiyama (Kyushu University, Japan)

**P-A1071** **Gradient metastability yields strong yet cryogenically tough additively manufactured steel**
Weiting Li (Tsinghua University, China)

| P-A0042 |

# Effect of austenite phase volume fraction on mechanical properties of hydrogen charged weld metals

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## Abstract

In recent years, there has been an increasing demand for applying high tensile strength steels to large structure constructions. However, cold cracking (hydrogen induced-cracking) is a serious trouble when high strength steels are welded. It has been known that this cracking resulted from diffusive hydrogen. Pre-heat treatment is carried out to prevent the cracking, but higher strength steels require strict temperature control. Therefore, we proposed a metallurgical solution, instead of pre-heat treatment, using duplex stainless steel containing an austenite phase, which has high resistance to hydrogen embrittlement. In this study, we investigated the hydrogen evolution behavior, visualization of hydrogen evolution sites, and the effect of diffusible hydrogen on the mechanical properties of weld metals with different volume fraction of the austenite phase. We developed weld metal with martensite and retained austenite based on Schaeffler's diagram. Microstructural observation was performed using optical microscopy. Hydrogen charging was conducted by the cathodic charging method under various conditions. Hydrogen embrittlement, the degradation of ductility was observed in the specimens with hydrogen. Thermal desorption analysis (TDA) and silver decoration technique revealed the effect of austenite phase on the hydrogen content and hydrogen evolution site in the weld metals.

**Keywords:** High strength steel, Duplex stainless steel, Austenite, Hydrogen evolution behavior, Mechanical properties

| P-A0070 |

# MIcrostructure control and stenghtening-toughening mechanism of 68.4GPa·% grade cold rolled steel

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## Abstract

A kind of medium manganese steel composed of Fe-6Mn-4Al-0.4C was designed. The effects of annealing parameters (temperature and time) on the microstructure evolution and mechanical properties after cold rolling were studied. With the increasing of annealing temperature , the yield strength decreased, the tensile strength first decreased and then increased, and the elongation first increased and then decreased. The mechanical properties change little with the increase of annealing time. The optimal heat treatment parameter of the steel after cold rolling is to hold the annealing temperature at 760°C for 30min, and then air cooling to room temperature. The tensile strength of the hot rolled specimens is 934MPa, the yield strength is 724MPa, the elongation is 73.3%, and the PSE reaches the highest value of 68.4GPa·%.

The microstructure evolution of the experimental steel mainly follows: carbide precipitate and redissolute with the formation of lamellar and equiaxed austenite and ferrite biphase structure. Lamellar grain transform into equiaxed grain, grain size coarse, austenite content increases, but transform into martensite due to the lack of stability. During the annealing process, the ferrite recrystallization occurs rapidly accompanied by the reverse austenite transformation, and the final microstructure changes to equiaxed morphology.

The stability gradient of austenite in annealed specimens causes discontinuous TRIP effect. Ferrite deformation, dislocation density and austenite stability affect work hardening behavior. The volume fraction and stability of austenite play an important role in the comprehensive mechanical properties.

**Keywords:** Fe-6Mn-4Al-0.4C steel, Intercritical annealing, Microstructure control, Strengthening-toughening mechanism

| P-A0082 |

# Effect of carbide coarsening behaviour on tensile properties of Cr alloying medium-Mn steel

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## Abstract

The coarsening behaviour of carbides in Cr alloying medium-Mn steel during critical annealing and its influence on mechanical properties were studied in this paper. The critical annealing (700°C) at different times (5min-10h) was carried out on Cr alloying medium-Mn steel after hot rolling, and the key factors affecting the strength and ductility of the test steel were analysed by uniaxial tensile test, multi-scale microstructure characterization, and theoretical calculation. The results show that, at the initial stage of critical annealing, carbides can reduce the lattice distortion of ferrite by absorbing C atoms, reduce the geometric necessary dislocation, and delay the tensile fracture (elongation from 16% to 19.4%). In addition, carbide precipitation strengthening makes up for the reduction of solid solution strengthening in the steel, so that the yield strength almost remains unchanged (about 740MPa). With the increase of critical annealing time, the further coarsening of carbide leads to the decrease of solution strengthening and precipitation strengthening, and the yield strength decreases continuously (from 743MPa to 350MPa). At the same time, the coarsened carbide becomes the priority point of crack nucleation, which leads to the premature fracture of the material in tensile deformation (elongation from 20% to 16.4%).

**Keywords:** Carbide, Medium-Mn steel, yield strength, fracture.

| P-A0084 |

# Heterogeneous ultrafine/fine-grained austenitic stainless steel: high strength and ductility

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## Abstract

Refining grain size is an effective method to improve the yield strength of austenitic stainless steels (ASSs) without significantly affecting its plasticity. This study aims to investigate the effect of annealing process on microstructural evolution and mechanical properties in phase reversion-induced ultrafine/fine-grained (UFG/FG) ASSs. The ASSs was warm rolled at 480°C to 70% thickness reduction, then cryogenic rolled to 80% thickness reduction and subsequently annealed at 770°C for 3-180s. The phase evolution and dislocation density changes were identified and measured by X-ray diffraction, and the corresponding microstructure was characterized by scanning and transmission electron microscopy and electron backscattering diffraction. The mechanical properties were determined by the room temperature tensile test. The results show that the heterogeneous UFG/FG structure formed in the initial stages of the reversion, but significant grain growth took place during the entire course of the reversion. The tensile strength (1228MPa) and yield strength (1065MPa) of the steel were greatly improved where the total elongation remained at the high level of 26.4%. In addition to solid solution and fine-grain strengthening, large strain gradients near UFG/FG interfaces are produced during deformation, which produces a significant back-stress to strengthen the material and to produce high back-stress work hardening for good ductility.

**Keywords:** Heterogeneous ultrafine/fine-grained ASSs, microstructural evolution, mechanical properties, back-stress work hardening.

# Corrosion Behaviors of U75vh, R350lht Heavy rail in Simulated atmosphere

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## Abstract

Along with the gradual deepening of modernization in our country, air pollution is increasingly serious, air corrosion has become an important factor affecting the service life of heavy rail, brought great losses and hidden dangers of safety to the railway industry for many years, but the first research on heavy rail steel anti-atmosphere corrosion has not reported. In this paper, the corrosion behavior of R350lht and U75vh heavy rail steel in simulated atmospheric environment is studied by using the cyclic infiltration corrosion test and the electrolysis method. The results show that the corrosion resistance of R350lht is obviously better than that of U75vh steel. The accumulation of Cr alloying element in the rust layer of R350lht steel promotes the rapid formation and content increase of the protective a-FeOOH phase in the rust layer, improves the ability of the rust layer to prevent the penetration of corrosive media, and can significantly improve the atmospheric corrosion resistance of heavy rail steel.

**Keywords:** U75vh, R350lht, heavy rail steel, corrosion behavior, simulated atmosphere environment

| P-A0147 |

# Effect of copper addition on the low-cycle fatigue behavior of ferritic heat- resistant steel at 630℃

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Topic area: Advanced Steels and Properties

## Abstract

To develop high-temperature materials used in the rotor/blade of the steam turbine, research on ferritic/martensitic heat-resistant steel has been actively conducted. Recently, 9-12% Cr steel with the addition of Mo and W has been developed for application in the 630 □ environments. Mo and W act as ferrite stabilizers and lead to solid solution strengthening and precipitation strengthening. Co is the key element in heat-resistant steel, leading to the enhanced creep resistance. Cu alloying can be a more economic alternative of the costly Co alloying because Cu can stabilize austenite and form Cu precipitates. Thus, the present work investigated the low cycle fatigue behavior at 630□ for the 3% Co, Cu-free steel and 2% Co, 1% Cu-added steel. Both materials showed tempered martensitic microstructure, and the prior austenite grain size of the Cu-added steel was slightly smaller that that of the Cu-free steel. Both materials showed an increase in cyclic softening with increasing strain amplitude. The Cu-free steel showed a slightly longer low-cycle fatigue life than the Cu-added steel. Detailed microstructure analysis was conducted to elucidate the observed low-cycle fatigue behavior of the two materials.

**Keywords:** Low-cycle fatigue, High temperature, Tempered martensite, Precipitates, Fractography

| P-A0203 |

# Effect of Microstructure on Mechanical Anisotropy of API X70 Linepipe Steels for Electrical Resistance Welding

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## Abstract

Rising global energy demand has caused the extension of natural gas and crude oil exploitation to remote areas and oceans, leading to the need of high-performance linepipe steels to withstand the extreme conditions of the different regions. Over the decades, thermo-mechanical control process (TMCP) has been developed to produce high-performance linepipe steels with high-strength and low-temperature toughness simultaneously. However, the API linepipe steels exhibit mechanical anisotropy because of asymmetric deformation during hot rolling. To fabricate the final product by electrical resistance welding (ERW) in the uniform elongation range, the mechanical anisotropy should be considered. This study aims to examine the correlation between microstructure and mechanical anisotropy, by varying the chemical compositions and process parameters of three high-strength API X70 linepipe steels fabricated through TMCP. The microstructures were characterized using SEM and EBSD analysis. Further, tensile and Charpy impact tests were conducted on the steel in different directions relative to the rolling direction. All steels indicated that higher strength and lower elongation in the T direction compared to the L direction because of the short dislocation glide path and ease of the pile-up at grain boundaries. The Charpy impact test results showed that the martensite-austenite (M/A) constituent can increase the ductile-to-brittle transition temperature (DBTT) by acting as a crack initiation site. In addition, the impact test specimens with T-L direction had a lower impact absorbed energy and higher DBTT compared to those with the L-T direction because the former exhibit fewer crack deflections at high-angle grain boundaries compared to the latter.

**Presenting author**

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**Keywords:** Linepipe steel, TMCP, Anisotropy, Impact toughness, Mechanical properties

| P-A0205 |

# Effect of Nb, Ti, and V additions on Hydrogen Embrittlement of Tempered Martensitic Low Alloy Steels

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## Abstract

Because of the increasing demands for hydrogen fuel to reduce the use of traditional fossil fuels, pressure vessel steels for storing and transporting hydrogen have been extensively studied. Because tempered martensitic low-alloy steel has a good combination of strength and ductility, it is a characteristic candidate material for pressure vessels. However, under prolonged exposure to hydrogen, this material exhibits a deterioration in its strength, ductility, and toughness, caused by hydrogen embrittlement (HE). The addition of micro-alloying elements such as Nb, Ti, and V, to the steel promotes the formation of various carbides during tempering heat treatment, resulting in a reduction in grain size and HE susceptibility. In particular, the MC carbide-matrix interface is known to act as irreversible trap sites with low hydrogen diffusivity, thereby significantly enhancing the HE resistance. Consequently, there is a need for studies on the HE mechanism and enhancement of HE resistance via micro-alloying element addition. In this study, three types of tempered martensitic low-alloy steels containing Nb, Ti, and V were quenched and tempered, and subsequently, their HE behaviors were evaluated using slow strain-rate test (SSRT) after electrochemical hydrogen charging. In-situ SSRT was also performed, and the results were compared with those of the ex-situ SSRT to investigate the effect of the hydrogen charging method on the HE behavior.

**Presenting author**

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**Keywords:** Tempered martensite, Hydrogen embrittlement, Micro-alloy, Slow strain-rate test

| P-A0231 |

# Development of 800MPa Grade Hot-Rolled High Strength Ferrite Steel with Excellent Ductility and Low Yield Ratio

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**Abstract:**

A tensile strength of 800MPa grade hot-rolled high strength ferrite steel with excellent elongation and low yield ratio was development, which can generate satisfactory combination of strength, ductility and weldability to meet the use to manufacture ERW high strength thin-walled square tube. The microstructure, precipitation behaviors, mechanical properties and strengthening mechanism of 800MPa grade hot-rolled high strength ferrite steel were investigated by utilizing optical microscope (OM), scanning electron microscope (SEM) and transmission electron microscopy (TEM). Titanium and molybdenum were added to 0.05% carbon and 1.5% manganese steel in order to lower austenite-Ferrite transformation temperature for fine carbides and to retard generating of pearlite and large cementite, respectively. Continuous cooling transformation diagrams determined by thermal simulation experiments showed that there were no pearlite at the cooling rate of 0.2 °C/s and the granular bainite occurs when the cooling rate reached 1 °C/s. Tensile strength of the tested steel increased with the coiling temperature decreases and it was achieved to 800MPa when coiling temperature was 600°C, the elongation and yield ratio were 24% and 0.86, respectively. Microstructure was ferrite and large amount of nano-precipitations with no pearlite and large cementite. The average size of ferrite is about 4.5μm, which is key to guaranteeing a low yield ratio. Fine carbides of 1~5nm in diameter were observed in the ferrite matrix of the tested steel, which are two different precipitation behaviors, one type is interphase precipitation that distributed in rows and formed at austenite-ferrite interfaces during transformation, and the other one is random dispersive precipitation that formed in coiling temperature. By energy dispersive X-ray spectroscopy, the size more than 50nm precipitates were Ti4C2S2 or TiC, the size below 10nm were TiMoC. The contribution of the precipitation strengthening to the yield strength of the tested steel has been estimated based on the Orowan mechanism.

**Key words:** 800MPa grade; high strength ferrite steel; nano-precipitation; strengthening mechanism; yield ratio

| P-A0295 |

# Effect of center segregation on low temperature impact toughness of welding heat-affected zone of pipeline steel

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## Abstract

The effect of center segregation on the low temperature impact toughness of the heat-affected zone (HAZ) of welded joints was studied by welding experiments on steel plates rolled from continuous casting billets with segregation grade of class 2 and class 3. The experimental results show that the HAZ of class 2 slab steel plate has more stable and excellent low temperature toughness than that of class 3 slab steel plate. The impact toughness of the HAZ of the class 3 slab steel plate is poor and has a certain fluctuation, and the delamination phenomenon is also observed in the fracture. The reason for this phenomenon is due to the enrichment of C and Mn elements in the central segregation zone. The formation of martensite microstructure with small grain size in the segregation zone leads to stress concentration, which is easy to form crack initiation and crack propagation path, and weakens the low temperature toughness of the joint.

Type or paste your text into this file, and use single-spaced 12-point Times New Roman. Paragraphs are justified (straight-edged) on both left and right. Leave a line gap between paragraphs. The limit for your abstract is 250 words. Do not include tables, formulae, and equations.

**Presenting author** must be identified in bold letters and underlined. Presenting authors, first name, surname, email address, and full mailing address must be included in the abstract. The email and mailing addresses of co-authors should be included in the abstract. Select the topic area in which you wish to make presentation at PRICM11.

The abstract deadline is Mar. 31. Authors will be informed about acceptance for presentation via email. Abstracts that do not meet these formatting requirements will be returned. The organizing committee reserves the right to edit abstracts for clarity or correctness of English.

**Keywords:** central segregation; heat-affected zone; in-situ microstructure; low temperature toughness.

| P-A0313 |

# Improvement of Impact Properties at Low Temperatures for 0.13C Cast Steel

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## Abstract

The Improvement of impact properties was performed for the cast steel containing 0.13C(JIS standard SCPL11) at a low temperature of 213K. The objective of this study is to satisfy the mean value of 18J on the absorbed energy for the low-temperature cast steel in the point of just usage of conventional static heat treatment equipment for low manufacturing cost. The heat treatment conditions consisting of homogenising, quenching and tempering process were investigated for the control of microstructures and mechanical properties for energy saving as the only heat treatment method.

The heat treatment consisting of the quenching at 1203 K for 14.4 ks followed by tempering at 983 K for 14.4 ks followed by air cooling was decided as a promising one, in the points of microstructure characteristics such as the suppression of primary α phase, complete tempering for curvilinear morphology and refinement of each phase. At 213 K, the average value in absorbed energy was 31.6J, which led to the satisfaction of initial objective value of 18J. Further, The brittle to ductile transition temperature was measured as 270 K, and the absorbed energy was measured approximately 132 J above 213K. In contrast, the values in YS, UTS and elongation at 293K were 440, 585MPa and 31.2% respectively, which resulted in the satisfaction of initial objectives, due to the microstructure control.

**Keywords:** impact value, energy saving process, low temperatures, heat treatment, low-carbon cast steel

| P-A0325 |

# A Study on the Improvement of Low Temperature Impact Toughness and Microstructure Changes of ERW X70 Steel Pipe

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## Abstract

In this study, we investigated the correlation between low-temperature impact toughness properties and microstructure of Electronic Resistance Welding (ERW) steel pipes under various welding conditions. We altered the heat input and Post Seam Annealing (PSA) temperature with high, medium, and low settings to examine their effects on microstructure and toughness properties. Microstructure analysis revealed a mixture of ferrite and pearlite under all conditions, with fine pearlite distributed at lower PSA temperatures and coarse-grained pearlite at higher PSA temperatures. Electron Back-scattered Diffraction (EBSD) analysis was employed to investigate the degree of recrystallization and residual stress due to PSA. Lower PSA temperatures displayed higher Low Angle Grain Boundary (LAGB) fractions, indicating incomplete recrystallization and high levels of residual stress. Higher PSA temperatures promoted grain growth and distribution of coarse-grained pearlite. We also conducted Penetrator analysis, a key factor known to affect impact toughness properties. Penetrator Area Ratio measurements revealed low fractions (0.004-0.007%) under all conditions. Elongated type Penetrators were identified as Si, Mn-rich Oxides, while Circular type Penetrators contained Ti, Nb, and MC carbides. Impact tests at -20°C were performed to examine low-temperature impact toughness properties based on the microstructure of ERW steel pipe welds. Results demonstrated superior impact toughness in samples with standard PSA temperatures, while the lowest PSA temperature samples exhibited inferior toughness, attributed to residual stress and abundant pearlite. The study further aimed to analyse the evolution of microstructures according to ERW welding conditions using a transmission electron microscope and associate the findings with impact toughness.

**Keywords:** Electronic Resistance Welding; X70 steel pipe; Penetrator; Low temperature toughness; Penetrator;

| P-A0703 |

# Analysis of Phosphating Defects for Hot-dip Zn-Al-Mg coated Steels

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## Abstract

The present study aims to study the defects for phosphated Zn-xAl-yMg (where x = 1.0~2.0 and 1.0~2.0 wt.%) hot-dip coated automobile steel plates which deteriorates significantly appearance quality and paint adhesion. The detect sample was prepared in painting pretreatment production line of a automobile manufacturer, and it was characterized using scanning electron microscope(SEM), and energy dispersive spectrometer(EDS). The results showed that the morphology of the phosphates at defect was extremely thin and flat, therefore the reflectivity of light was improved. Such defect was named as white spot for brighter appearance in macroscope. Removing phosphating film with a concentration of 50g/L Cr2O3 at 75 oC for 15 minutes, Zn-Al-Mg coatings were analysed with SEM, EDS, and X-ray photoelectron spectroscope (XPS). Trace amounts of Si element present at the defect. Silicates are usually added to the degreasing solution to protect the substrate from corrosion by alkaline solutions. Take the on-site degreasing solution back to the laboratory, and use a filtration device to cellect the insoluble substances inside. Through SEM, EDS and XRD analysis of the substance, it was found that it contained a large amount of silicon oxides. Finally, the defect maybe caused by the silicic acid hydrolysate in the degreasing solution adhering to the surface of the Zn-Al-Mg coating, which inhibits the normal growth process of phosphates.

**Keywords:** Zn-Al-Mg coatings; phosphating; painting pretreatment process; scanning electron microscope; X-ray photoelectron spectroscope;

| P-A1070 |

# Effect of core-shell type second phase formed by interrupted-quenching and intercritical-annealing on mechanical property in a medium manganese steel

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## Abstract

Medium manganese steels, which are expected as the next-generation high-strength steel sheets for automobiles, contain retained austenite stabilized by Mn and C in the microstructure. The retained austenite leads to an excellent strength-elongation balance of this type of steels due to the TRIP effect. However, since sufficient strength cannot be obtained simply by quenching and tempering (intercritical annealing), cold or warm working is usually performed before the intercritical annealing to increase yield strength by grain refinement. However, it would be difficult to perform cold or warm working of hard martensite in the actual process. In contrast, the interrupted-quenching and intercritical-annealing (IQ-IA) process proposed in this study aims to simultaneously increase the strength and elongation of medium-Mn steels by heat treatment alone, without using working. Specifically, Fe-5Mn-0.1C alloy was subjected to interrupted quenching to a temperature between Ms and Mf followed by intercritical annealing in the ferrite and austenite dual-phase region at around 923 K. As a result, a core-shell type second phase, which consisted of a fresh martensite core surrounded by a film-like retained austenite shell, was formed. The resulting steel is strengthened by the fresh martensite core and its ductility is improved by the TRIP effect of the film-like retained austenite shell. Characteristics of the microstructure and mechanical properties of the medium Mn steel with core-shell type second phase will be introduced.

**Keywords:** Medium manganese steel, microstructure control, retained austenite, element partitioning, mechanical properties

| P-A1071 |

# Gradient metastability yields strong yet cryogenically tough additively manufactured steel

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**Abstract.**

Additively manufactured steels usually exhibit an excellent synergy of strength and ductility due to their unique ultrafine hierarchically heterogenous microstructure. Yet, their toughness, in particular cryogenic toughness is intrinsically inferior as the formation of micro-voids and oxide inclusions can hardly be fully prevented during additive manufacturing. Here, we deploy a gradient metastability strategy to make additively manufactured steels strong yet cryogenically tough. As demonstrated in a maraging stainless steel, cryogenic (77K) impact toughness can be enhanced by three times without a sacrifice of strength via tailoring chemically gradient metastable austenite in the ultrastrong hierarchically martensitic matrix. This unique gradiently stable austenite could not only absorb massive energy via deformation induced martensite transformation but also make a remarkable contribution to local stress alleviation, crack passivation and deflection. Gradient metastability strategy can be potentially applicable to other additively manufactured alloys, and expands the dimensionality of designing untrastrong yet cryogenic tough alloys.

**Keywords:** Selective laser melting, Cryogenic toughness, Metastable austenite

# POSTER Session 2

## Symposium B : Advanced Processing of Materials

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| P-B0056 |

# Application of Green Manufacturing Technology in ASP1700 Hot Rolling Production Line

Wei Xiudong, Wu You, Qi Man, Xu Xiaoke

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**Abstract:**
The ASP1700 hot rolling production line of Chaogang Iron and Steel adopts green manufacturing technology, achieving better energy-saving and carbon reduction effects. The heating furnace mainly adopts vaporization cooling, black body enhanced radiation heat transfer technology, and low nitrogen burner combustion technology to reduce mixed gas fuel consumption and achieve carbon and nitrogen reduction. The rolling process uses hot delivery and hot charging technology and low-temperature rolling technology to improve the comprehensive yield. The slab hot delivery and hot charging rate increased by 12% compared to the plan, the comprehensive yield rate increased by 0.02% compared to the plan, and the oxidation burn loss rate decreased by 0.03%. The process energy consumption met the company's challenge. The consumption of high and coke mixed gas and power consumption decreased by 0.03GJ/t and 4kwh/t respectively compared to the actual completion in 2021, reaching the best level in the history of the production line.

**Key words:** hot rolling; heating furnace; Green manufacturing technology; Low nitrogen combustion; Hot charging and hot delivery

| P-B0139 |

# Influence of Cooling Parameters on Precipitation of Grain Boundary Cementite of 0.92%C Steel Wire Rods

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## Abstract

Drawability is an important property of cord steel wire rods to ensure the productivity of steel wire. The grain boundary cementite(GBC) has harmful influence on the drawability of steel, which is normally strongly related to carbon content, center segregation and cooling rate after laying. Because of the high carbon content and existence of severe center segregation, the control of GBC of 0.92%C steel wire rods usually requires a high cooling rate, which leads to high strength and low drawability. Thus a new method is needed to prevent the precipitation of GBC. In this paper, the influence of deforming and cooling parameters on precipitation of GBC of 1.15%C steel was studied. The carbon content corresponds to 0.92%C wire rods with a center segregation index 1.25. The results show that the cementite precipitation temperature range of specimens without deformation decreases from above 950°C to 900°C-950°Ccompared to specimens with compression of 30%. The reason is that the austenite of the specimens without deformation has higher stability due to bigger grain size and less crystal defects like dislocations etc., the cementite precipitation temperature is delayed to a lower range which decreases the growing rate and amount of GBC. Therefore, a higher laying head temperature and longer holding time in high temperature range was applied to the industrial experiment of 0.92%C wire rods to fully release the deformation energy accumulated in the rolling to prevent the precipitation of GBC. The penalty point of GBC decreased dramatically from 42 to 22.

**Keywords:** high-carbon steel wire rods, segregation, GBC, precipitation

| P-B0158 |

# Shape optimization of large metallic hydrogen permeable membranes and development of forming technology

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## Abstract

As a means of producing high purity hydrogen, the development of hydrogen separation membranes using alloys is under way. So far, hydrogen permeable membranes using Pd and Pd alloys have been partially put into practice. However, because Pd is a rare and expensive resource, the development of hydrogen permeable membranes using V alloys, which are inexpensive and easily available, is promoted. For large-scale hydrogen production and high efficiency, it is desirable to use thin, flat membranes, which can be created by rolling as a material for permeable membranes. However, there is a problem of wrinkles and cracks occurring during or after hydrogen permeation in thin large diameter membranes. It is considered that the stresses acting in the membranes are complexly affected by factors such as deformation due to hydrogen pressure during hydrogen permeation, thermal expansion due to heat, and lattice expansion due to dissolved hydrogen during hydrogen permeation. Therefore, to improve the durability of large-diameter thin membranes, it is necessary to quantitatively evaluate the factors that cause stress and consider damage suppression measures that can reduce stress. In this study, we investigated the effects of imparting a three-dimensional shape to hydrogen permeable alloy membranes on the deformation behavior and stress distribution of the membranes during hydrogen permeation using FEM analysis that simulated hydrogen pressure, thermal expansion, and lattice expansion due to dissolved hydrogen. Furthermore, we developed a forming method for thin permeable membranes to achieve the optimal shape.

**Keywords:** Hydrogen permeable membrane, Vanadium alloy, Hydrogen-induced lattice expansion, Finite element method, Deep drawing

| P-B0167 |

# Data assimilation integrating phase-field simulations and X-ray imaging for highly accurate prediction of columnar dendritic growth

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## Abstract

An accurate understanding of the dendrite growth process is essential for improving the quality of casting products. Phase-field simulations and time-resolved X-ray tomography are among the most powerful numerical and experimental tools as state-of-the-art techniques for evaluating the dendrite growth process. However, these technologies have limitations due to the lack of material properties and spatiotemporal resolutions. Integrating phase-field simulations and X-ray imaging through data assimilation are promising research fields as the shortcomings of each method are substantially addressed.

In this study, we have developed a data assimilation system using solid fraction data in the direction of X-ray projection. We validated the developed data assimilation system through twin experiments for columnar dendrite growth in a thin film and cylinder. These twin experiments were related to the data assimilation method using experimental two- and three-dimensional X-ray imaging results. We also attempted data assimilation using these actual experimental results. Since the computational cost is extremely high in the data assimilation system, we accelerated data assimilation computation by using the adaptive mesh refinement method and parallel computing with multiple graphic processing units for phase-field simulation and the local ensemble Kalman filter.

**Keywords:** Phase-field simulation; Data assimilation; X-ray imaging; Columnar dendrite growth

| P-B0372 |

# Effects of Heat Treatment in Hydrogen Environment on Hydrogen Permeability of Pd-40mass%Cu Alloy Membrane

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## Abstract

Pd-40 mass% Cu alloy membranes with a B2 crystal structure are in practical use as hydrogen-permeable membranes for hydrogen separation and purification, yielding ultra-high purity hydrogen. The typical operating temperature of this alloy membrane is around 623-723 K, but due to the low activation energy of hydrogen permeation, the alloy is expected to exhibit a relatively high hydrogen permeation capacity even at low temperatures below 473 K. However, hydrogen permeability performance at low temperatures has not been fully investigated. Previous studies have shown that the temperature dependence of hydrogen permeability exhibits a linear relationship following the Arrhenius equation at temperatures above 473 K. Below 473 K; however, the linear relationship deviates, and a significant decrease in permeability is observed, especially near room temperature, which is probably because defects in the material trap hydrogen at low temperatures.

On the other hand, the crystal structure of Pd-40 mass% Cu alloy after melt and rolling is an FCC (face-centered cubic) phase, so heat treatment is required for B2 transformation. This heat treatment is conventionally performed in a reducing hydrogen atmosphere, but the effect of the hydrogen during heat treatment on the hydrogen permeability of Pd-40 mass% Cu alloy is unknown.

In this study, Pd-40 mass% Cu alloy films with an FCC phase were heat-treated in different hydrogen pressure environments to investigate the effect of the hydrogen atmosphere during heat treatment on hydrogen permeability. As a result, the hydrogen permeability of the films annealed in hydrogen above 400 kPa was reduced compared to those annealed in hydrogen below 300 kPa. Also, the diffraction peaks of the samples annealed above 400 kPa were shifted to the higher angle side, indicating lattice contraction. These results suggest that hydrogen-induced vacancies are generated during heat treatment in a high-pressure hydrogen atmosphere.

**Keywords:** PdCu alloy membrane, CsCl-type crystal structure hydrogen permeability, hydrogen diffusivity, hydrogen trapping

# Crystal growth of long Ru-Mo-W alloy single crystal wires by the dewetting micro-pulling-down method equipped with a continuous feeding system

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## Abstract

Recently we have developed a novel resistance heating wire that improves energy efficiency in the deposition of organic electroluminescent thin films by vacuum evaporation. Using the dewetting micro-pulling-down (μ-PD) method, a high-speed single-crystal growth method, we have developed a Ru-Mo-W alloy (Ruscaloy) wire with a lifetime at 1873 K ~3 times longer than that of conventional Ta wire, and with high electrical resistivity and toughness [1]. The micro-drawing method allows single-process production of difficult-to-process alloy wire rods with a footprint of less than 10 m2, however, the length is limited to around 10 m in batch production. The μ-PD method can produce alloy wires in a single process; however, in batch production, the length is limited to ~15 m, and macro segregation can occur. In this study, we aimed to produce homogeneous and long single-crystal wires by stabilizing crystal growth conditions with the continuous feeding system.

A Ru60Mo15W25 alloy wire was grown using a dewetting μ-PD furnace, equipped with a developed continuous feeder with a feedback system. Rod-shaped alloy was continuously fed following the crystal growth to produce a wire rod with a diameter of 0.8 mm and a length of ~33 m. The composition of the samples annealed at 2273 K for 3 h was analyzed by WDX, and the average compositions over a length of 30 m were W: 25.86±0.088 at%, Mo: 14.35±0.036 at%, indicating that the compositional variation was significantly small.

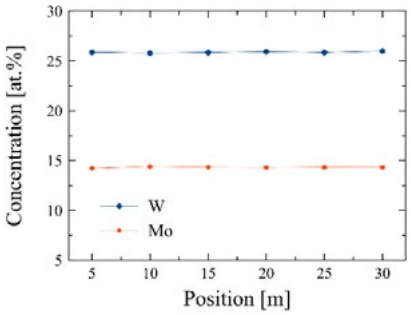



**Fig.1** The compositions of W and Mo in the longitudinal direction of the grown wire.

[1] R. Murakami, A. Yoshikawa et al., Int. J. Refract. Met. Hard Mater. 114 (2023) 106235.

**Keywords:** Ruthenium alloys; Refractory alloys; Single-crystal growth; Organic light-emitting diodes; Resistive heating element

| P-B0923 |

# Synthesis of high purity titanium nanopowders by high-energy ball milling of titanium hydride

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## Abstract

Titanium (Ti) has the characteristics of a high strength-to-weight ratio, excellent corrosion resistance in seawater, and ease to alloy with elements such as Al, V, and, Mo, that of appropriate for applying in the automotive and aerospace industries. Using the casting process can produce complex part geometries but is challenging for Ti due to its relatively high melting point and fatal drawbacks in oxidation. Hence, the powder metallurgy technology is generally applied to fabricate complicated shaped parts having a homogeneous composition. In order to make a fully densified Ti-base product, the initial Ti powder should be small in size and contain as low an oxygen level as possible. Fine Ti powder is prepared by a high-energy ball mill process, but it is difficult to obtain a uniform shape and highly purified powder due to the ductility and oxidation characteristics of Ti. To solve these problems, we attempt to use TiH2 powder having inherent brittleness for obtaining the nano-sized TiH2 by milling in a relatively short time, and then oxidation-suppressed pure Ti nanopowder is synthesized through a dehydrogenation process of ball-milled powder. In addition, to optimize the milling time, the characteristics of the powder milled at 500 rpm for various times using zirconia balls with a diameter of 0.3 mm were analyzed. The prepared powder showed a size of 200 nm, and through analysis such as X-ray diffraction, differential thermal gravimetry, scanning electron microscope, optimal process condition for the production of high-purity Ti nanopowder is suggested.

**Keywords:** Titanium hydride, High-energy ball milling, Dehydrogenation, Pure titanium

| P-B0926 |

# Macroporous structures tailored via various sublimable vehicles in freeze-casting process

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## Abstract

Porosity has been known to be a negative effect on densification, but it constantly is receiving attention due to the synergistic effects between pores and metal- or ceramic-base matrices such as low density, high surface area, thermal or electrical insulation, permeability, and good adsorption of electromagnetic waves that do not appear in dense bodies. Meanwhile, since the porous body exhibits various physical properties depending on the pore shape and size, there have been numerous attempts to develop pore formation methods for modifying the pore characteristics precisely. Among them, a freeze-cast method that uses slurry mixed with solid powder has been regarded as an appropriate technique for manufacturing due to its merits of process simplicity and no restriction on solid powder. In this regard, we focus on the tailoring of directionally aligned pore structures using various sublimable vehicles such as tert-butyl alcohol (TBA) and H2O. The porous preform is fabricated by a freeze-cast method using TBA base slurry with various dispersing agents and binders. The prepared slurry is poured into Teflon and copper cylinders, then immersed into cooled ethanol for directional solidification of sublimable vehicles. Aligned pores are generated by the sublimation of solvents during freeze-drying. Finally, the porous green body is consolidated through a two-step sintering process. The sintered preforms show different pore sizes, morphologies, and surface roughness depending on the freezing temperature, drying condition, and sublimable vehicle. Consequently, we suggested a feasible technique for precisely controlling the porosity microstructures through freeze casting.

**Keywords:** Freeze casting, Pore structure, Tert-butyl alcohol, Microstructure

| P-B0970 |

# Improved toughness of warm-rolled medium-Mn steels through nano-sandwich microstructure

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## Abstract

Here, we tried to improve the toughness of medium-Mn steels through implementation of nano-sandwich microstructure via warm rolling. The hot-rolled and annealed (HRA) specimen shows the martensite and austenite with multi-variant laminate morphology. The warm-rolled (WR) specimen exhibits similar microstructure and phase fraction with HRA, however, it indicates the single directional laminate structure, which is aligned to rolling direction. The resulting microstructure is called nano-sandwich structure. The HRA shows the poor toughness, because the crack propagated rapidly along the prior austenite grain boundaries (PAGBs) weakened by Mn segregation. However, WR showed improved toughness relative to HRA, because the cracking is suppressed by breaking of PAGBs during warm deformation. Furthermore, the crack could propagate in a direction perpendicular to the crack propagation, reducing the propagation energy and increasing the toughness; this phenomenon is called delamination. Therefore, it is expected that warm rolling is suggested as novel route for damage tolerant microstructural design of medium-Mn steel.

**Keywords:** Warm rolling, Medium-Mn steel, Nano-sandwich microstructrure, Impact toughness, Prior austenite grain boundary.

| P-B0982 |

# Comparative Study of Self-Piercing Riveting and Spot Impact Welding for Dissimilar Al/Steel materials

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## Abstract

Vaporizing foil actuator welding (VFAW), a high-velocity impact welding technique was utilized to achieve dissimilar joining of SPFC DP590/AA5052 materials. The mechanical and fatigue characteristics of the joints were evaluated using lap-shear testing, cross-tension testing, fatigue testing, microhardness measurements, optical imaging. The obtained results were then compared with those of self-piercing riveting (SPR) joints.

The results demonstrated that VFAW joints exhibited enhanced strength and energy absorption in comparison to self-piercing riveting (SPR) joints. Fatigue resistance was found to be similar between VFAW and SPR. Microhardness measurements conducted on VFAW and SPR joints indicated consistent hardness values along the entire length of the weld, indicating the absence of a heat affected zone. The fatigue strength is primarily influenced by the shape and type of notch that forms at the end of the nugget. The VFAW mechanism was further analyzed by observing the interface between the joined materials.

**Key Words:** Self Piercing Riveting, Vaporizing Foil Actuator Welding, Al/Steel dissimilar materials, Mechanical properties, Fatigue.

| P-B1170 |

# Acoustic Field-Enabled Intelligent Air Conditioning for Ultrafine Dust Reduction in Smart Buildings

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## Abstract

Fine particles in polluted air pose significant challenges to human safety and building energy consumption. Conventional technologies, such as physical filters, electrostatic adsorption, and ionic adhesion cannot mitigate fine dust from metal particles and harmful gases. This study explores a novel approach utilizing an acoustic field with optimized sound frequency and pressure to reduce fine dust in industrial environments. This method significantly increases the size of ultrafine dust, causing priority pressure differences in the air conditioning system and maintaining the pressure differential for an extended period, thereby saving overall air conditioning costs. The study involved installing two laser scattering-based fine particle measuring instruments within a department store's air conditioning system. For the ultrasonic aggregation system design, one instrument was installed in the air conditioning system (Device1), and another was placed in a chamber (Device2) to measure fine dust particle distribution between 0.3 μm to 10 μm over a specific period. The fine dust measurement system comprised a monitoring display panel, IoT communication module, and laser scattering-baser fine dust particle sensor. The IoT communication module used long-range Wi-Fi frequencies or router/ethernet cables. It was designed to enable continuous data communication using commercial systems such as USIM chips. As a result, at 100 dB and 53.125Hz, the fine dust (PM2.5) reduction efficiency reached approximately 99% after 5 minutes, representing a significant improvement over the natural decay condition. The results suggest that this innovative technology can significantly improve indoor air quality in large-scale multi-use facilities while minimizing energy consumption. It addresses the urgent need for efficient ultrafine dust removal in intelligent buildings, contributing to better facility management and human safety.

**Keywords:** Acoustic Field, Intelligent Air Conditioning, Particle Aggregation, Smart Buildings, Ultrafine Dust.

# POSTER Session 2

## Symposium C : Structural Materials for High Temperature

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**P-C0933** **Fabrication of W-Cu composite powders by ball milling and hydrogen reduction of WO3-CuO powder mixtures**
Ji Won Choi (Seoul National University of Science And Technology, Korea)

| P-C0109 |

# Liquation cracking temperature range of repair weld heat-affected zone for long-term aged 247LC superalloy evaluated by Varestraint test

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## Abstract

In this study, the liquation cracking temperature range(LCTR) of long-term aged 247LC superalloy repair welds was quantitatively evaluated using spot-Varestraint testing, especially for application in the repair weld heat-affected zone(HAZ). Overaging heat treatments at 1,000 □ for times up to 3,000 h were used to simulate long-term serviced materials. The metallurgical mechanism of the evaluated liquation cracking susceptibility of the over-aged 247LC superalloys was clarified by analyzing the microstructural characteristics at the liquation cracking surface and thermodynamic calculations. From the spot-Varestraint tests for the over-aged materials, the LCTR were all evaluated over 420 K. Compared to the LCTR of pre-weld heat treated 247LC (65 K), these results demonstrate that the over-aged 247LC superalloy face significantly serious liquation cracking susceptibility in repair weld HAZ. Based on local element distributions at the liquation cracking surface analyzed by transmission electron microscopy and Thermo-Calc calculations, the underlying metallurgical mechanism of high LCTRs of over-aged materials could be identified as precipitation of MC and M6C carbides during the over-aging treatment. In other words, the cracking was attributed to the constitutional liquation of the MC and M6C carbides, which promoting local liquation at the interface between the γ phase at lower temperature than the equilibrium solidus (1530 K) of the 247LC. The estimated liquation initiation temperatures at the MC/γ and M6C/γ interfaces are 1125 and 1420 K, respectively. The LCTRs expansion behavior of over-aged materaials were examined as a result of quantification of carbide, and a high relationship between LCTRs and carbides fraction was confirmed.

**Keywords:** 247LC superalloy, Overaging, repair welding, liquation cracking, spot-Varestraint test

| P-C0215 |

# Quantitative analysis and formation mechanism of inclusions in a vacuum induction melted Ni-Co based superalloy

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The development of aerospace industry promotes the improvement of thrust-weight ratio and the operation temperature of aero-engine and gas turbine as well as the evolution of Ni-based superalloys for higher mechanical properties at elevated temperatures [1-3]. GH4068 alloy is a γ'-Ni3(Al,Ti) precipitation strengthened wrought superalloy with higher service temperature, which is regarded as a potential material for turbine disk of aero engines [1]. High content of Co promotes the formation of a more stable microstructure and Ti enhances the effect of phase interface strengthening by substituting Al atom in γ' phase. In addition, the high level of Al+Ti+Nb and Ti/Al ratio increases the antiphase domain boundary energy, which is also beneficial for the improvement of high temperature mechanical properties. In general, the GH4068 ingots are prepared by the triplex melting process, viz. vacuum induction melting (VIM) plus electroslag remelting (ESR) and vacuum arc remelting (VAR) [3]. Moreover, VIM plus electroslag remelting continuous directional solidification (ESR-CDS) and VIM plus electron beam smelting (EBS) are also used for the preparation of GH4068 ingots [4, 5]. As the master alloy for multiple melting process, the type, content and distribution of inclusions in the VIM ingot are crucial to the purity of alloy.

Generally, metallographic method and bulk sample electrolysis method are commonly used for inclusion analysis in superalloys [6]. The metallographic method requires manual acquisition of inclusion parameters, including the type, content, distribution and chemical composition of inclusions, in a large field of view. It is difficult to obtain the statistical results of inclusion for superalloys since the contents of impurity elements as well as nonmetallic inclusions are low [7-9]. On the other hand, the reliability of bulk sample electrolysis method for superalloys is low since the separation of inclusions from superalloy matrix is incomplete, although the statistical significance for the bulk sample electrolysis method is higher than that of metallographic method [6]. The automatic scanning electron microscope analysis system for inclusions, which is developed by the ASPEX Corporation and Oxford Instruments, can automatically analyze the inclusions in a large area and obviously improves the efficiency of inclusion analysis [10, 11]. However, the systems as mentioned above are mostly used for the analysis of inclusions in iron and steel. Limited data have been published on the analysis of inclusions in superalloys for the reason that the inclusion analysis module, which is applicable to superalloys, has not been established.

The present research aims to quantitatively characterize the inclusions in GH4068 alloy prepared by vacuum

induction melting employing the automatic analysis system for inclusions and self-designed superalloy inclusion analysis module. The thermodynamic analysis of inclusion formation was performed and the effect of oxygen/nitrogen content on the number densities of inclusions were summarized.

The inclusions in the GH4068 ingots mainly include oxides, carbides, nitrides, carbonitrides and complex inclusions. The oxides are mainly concentrated in the top center of the cast ingots, and the nitrides and complex inclusions are mainly distributed near the bottom and edge of ingots. The homogeneous nucleation of Al2O3 is spontaneous during the solidification although TiN prefers to wrap on the nucleated particles. The increase of oxygen/nitrogen content results in the increase of oxides, nitrides and complex inclusions, while N shows negligible influence on nitride inclusions formation when its concentration is higher than 3 ppm.

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| P-C0317 |

# Influence of cellular structure on mechanical properties of Ni-based superalloy fabricated by metal 3D printing

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## Abstract

Ni-based superalloys that exhibit high strength at high temperatures and excellent oxidation resistance are used for turbine blades of an aircraft engine. In recent years, it has been reported that the nano-scaled cellular structure is formed in the alloys fabricated by laser beam powder bed fusion (LB-PBF) which is one of the additive manufacturing technologies. The alloys with the unique microstructure show excellent mechanical properties. However, the influence of process conditions on the morphology of the cellular structure has not been clarified in detail. In addition, the relationship between the morphology of cells and mechanical properties has also not been investigated yet.

In this study, the influence of input energy density on the morphology of the cellular structure in Inconel 718 alloys fabricated by LB-PBF was evaluated, focusing on the cell spacing. In addition, its effect on the strength of the alloys at room temperature were examined. We found that the cell spacing increases with increasing the energy density. Moreover, microstructure observation using a transmission electron microscope revealed that the dislocation cell with accumulated dislocations is formed at the interfaces of the cellular structure. It is supposed that the dendritic solidification with a very fast solidification rate is responsible for the formation of the fine cells. We also found that the tensile strength of the alloys depends strongly on the cell spacing. The alloys with the cellular structure exhibit approximately 15% higher hardness that the conventional solution treated alloys.

**Keywords:** Additive manufacturing, Laser beam powder bed fusion, Cellular microstructure, Mechanical property

| P-C0334 |

# Characterization of microstructure of tantalum/steel interfaces prepared by explosive welding and its thermal cyclic characteristics

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## Abstract

Tantalum alloys are often used as clad materials to protect steels used in high-temperature oxidation/corrosion environments in industries such as power generation, aerospace, and defense due to their high melting point (>3000°C) and excellent wear and corrosion resistance. Explosive welding is used to manufacture double-layer pipes with Ta alloy clad onto the inner surface of Fe-based steel pipes because Ta has a high melting point compared to Fe. The microstructure and mechanical integrity of the Ta/Fe interface vary with the explosive welding process parameters, affecting the pipe's durability during thermal cycles caused by start-up/shut-down procedures. Therefore, this study investigated the microstructure and mechanical integrity of the Ta/steel interface under different explosive welding conditions and examined the microstructural changes of the interface caused by thermal cycles. Scanning electron microscopy observations showed that weaker explosions resulted in low-amplitude wavy interfaces and intermixed zones (IMZ) without a vortex, while stronger explosions produced high-amplitude wavy interfaces with a vortex caused by Ta/Fe mixing. The vortex-melted zone (VMZ) was observed inside the vortex in the high-amplitude wavy interface. Transmission electron microscopy analysis confirmed that the VMZ was amorphous caused by mixing Fe and Ta due to high-speed impact energy, followed by rapid cooling by surrounding cold Ta alloy. The shape of the vortex and the distribution of the VMZ are important factors during thermal cycles due to the large difference in the thermal expansion coefficient between Ta and Fe, and they should be studied in connection with phase transformation behavior.

**Keywords:** Explosive welding, Ta/steel dissimilar metal, Interface, Microstructure, Thermal cycles

| P-C0587 |

# Formation mechanism of special grain boundary and the effect on properties of a Fe-Ni-base superalloy under hot deformation

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## Abstract

The Fe-Ni-based superalloy is widely utilized for hot section components such as industry gas turbine (IGT) wheels, where excellent elevated temperature properties and environment resistance are required. Considering the significance of the microstructures for industrial applications, so far research activities in this field have been mainly aimed at DRX or strengthening phase control during hot deformation. Nevertheless, the final morphology of grain is greatly affected by the growing process, which affects the mechanical properties of the alloy. Therefore, it is necessary to explore the grain growth mechanism under different hot deformation conditions. After heat treatment at 980 °C, the alloy forged at 1010 °C was completely recrystallized after holding for 2 min, and the grains growth uniformly with the process of holding. After holding for 30 min, the alloy was completely recrystallized that forged at 1110 °C, showing a special microstructure with zigzag grain boundaries and small grains within large grains. The grain boundaries of small grains are all composed of Σ3, while the orientations of large grains are only fixed. This microstructure increases the stress rupture life of the alloy by 67% compared forged at 1010 °C. The findings help to understand the formation mechanism of special grain boundary of superalloy during microstructure evolution under hot deformation, and are also beneficial for optimizing the microstructure to control the required properties for manufacturing IGT wheels.

**Keywords:** Fe-Ni-based superalloy, Hot deformation, Grain growth, Stress rupture property

| P-C0653 |

# Numerical Simulation and Experimental Study of Electroslag Remelting Process (ESR) for Φ1100mm Ni-Based Superalloy Ingot

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## Abstract

With the development of heavy-duty gas turbines, the use of GH4706 superalloy has necessitated the manufacturing of larger and larger initial blanks. Enlarged ingot types inevitably face issues such as element distribution, freckles, and other defects, which usually occurred during the solidification front. Numerical simulation provides a fast and effective method for studying the motion state and morphology of the melt pool in the electroslag process to reduce the generation of metallurgical defects. In this study, numerical modelling was employed to investigate the entire electroslag remelting (ESR) process of a Φ 1100 mm GH4706 superalloy. The predicted model of 2D axisymmetric, coupled with multiple physical fields, was constructed to calculate the flow field, temperature field, melt pool shape, and solidification structure throughout the ESR process. The results showed that the molten pool exhibited two clockwise flow fields, influenced by buoyancy and Lorentz forces. With an increase in melting speed, the metal molten pool continued to deepen, resulting in an increased growth angle of dendrites. This also indicated the reduction in the average grain area and radius of the ingot, as well as enhance the effect of the grain refinement. Meanwhile, the local solidification time (LST) was also calculated using different melting speeds, and the melting pool depth and solidification structure were validated through industrial experiments. The combination of numerical simulation results and industrial ingot analysis experiments showed good agreement, confirming the accuracy of the thermal history and solidification microstructure calculations throughout the melting process.

**Keywords:** Numerical simulation; Electroslag Remelting; solidification structure; GH4706 superalloy

| P-C0855 |

# Stress rupture properties and deformation mechanisms of a Re-low second-generation Ni-based single crystal superalloy

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## Abstract

The microstructure and deformation mechanism of a second-generation nickel-based single crystal superalloy containing 1.5 wt.% Re were investigated by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) after stress rupture at 982 °C/248 MPa and 1038 °C/172 MPa. During stress rupture deformation, the γ′ phase coarsens and connects, forming an N-type rafted structure perpendicular to the stress axis, and the distortion extent of γ′ phase increases with the distance from the fracture. Compared with 982 °C/248 MPa, the distortion extent of γ′ phase after ruptured at 1038 °C/172 MPa is greater. a<010> superdislocations and a few uniform interfacial dislocation networks were found after rupture at 982 °C/248 MPa. After stress rupture at 1038 °C/172 MPa, dislocation networks, K-W locks and denser dislocation networks became the typical feature. More regular and denser dislocation networks can prevent matrix dislocations shearing into γ′ phase, thus improving the creep resistance of the alloy.

**Keywords:** nickel-based single crystal superalloy, rated γ′ phase, stress rupture property, deformation mechanism

| P-C0920 |

# Synthesis and characterization of W-Ni-Cu alloys using metal oxide powders

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## Abstract

Tungsten (W) is considered one of the suitable materials for radiation fields and high-temperature applications due to its high atomic numbers and excellent thermal properties such as high strength for high temperature, extreme melting point, and low thermal coefficient. However, there are inherent limitations in use because of its high ductile-to-brittle transition temperature, poor ductility, and low sinterability. Meanwhile, tungsten heavy alloy (WHA), obtained by adding alloying elements such as Ni and Cu to W, presents unique properties which are high hardness with improved sinterability, thermal conductivity, and corrosion resistance. The WHA powder is simply fabricated by high-energy ball milling of elemental metal powders, but it has fatal problems for contamination by milling media and the formation of hard aggregates during the process. Recently, an interesting study has been reported about the preparation of WHA powder by high-energy ball milling using metal oxides instead of metals and subsequent hydrogen reduction of their mixtures. This method is efficient for minimizing impurities and suppressing the formation of large aggregates. Therefore, this study aims to synthesize a homogeneous W-Ni-Cu heavy alloy powder by high-energy ball milling and hydrogen reduction of WO3, NiO, and CuO powder. And then, prepared W-Ni-Cu powder is consolidated by pressureless sintering under a hydrogen atmosphere. The characteristics for the sintered body are analyzed by XRD, SEM, EBSD, and the relations between microstructure and properties are discussed.

**Keywords:** WO3-NiO-CuO powder mixture, W-Ni-Cu alloy, hydrogen reduction, microstructure

| P-C0930 |

# Effect of thermal compression temperature and deformation on abnormal grain growth of solution treated GH4096 alloy

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## Abstract

The effects of thermal compression temperature and deformation on the abnormal grain growth of GH4096 alloy after solution treatment were studied by thermal compression tests combined with numerical simulations. Experimental results show that after 1075 °C solution heat treatment, abnormally grown grains were found in the arc-shaped strip areas near the top and bottom of samples compressed at 1060 °C and 1080 °C respectively. EBSD analysis was utilized to study the grain orientation and local misorientation distributions in the arc-shaped strip areas of 1060 °C-compressed sample before and after 1075 °C solution heat treatment. The results show that there is deformation dead zone, critical deformation zone and recrystallization zone in the compressed sample. The deformation dead zone undergoes low deformation stress, and the deformation stress and grain structure remain unchanged after heat treatment. The critical deformation zone possess high deformation stress. After heat treatment, the deformation stress significantly decreases and the grains grow abnormally with an average grain size of ASTM4. The recrystallization zone has low deformation stress. In the forged state, the grain size of the recrystallization zone is larger than that of the deformation dead zone and critical deformation zone. After heat treatment, the deformation stress decreases and the average grain size turns into ASTM9. According to the numerical simulation results, the strain level of the circular arc strip area of the sample compressed at 1060 °C and 1080 °C following 1075 °C solution heat treatment is about 0.113 and 0.188 respectively.

**Keywords:** GH4096 alloy; Solution heat treatment; Abnormal grain growth

| P-C0933 |

# Fabrication of W-Cu composite powders by ball milling and hydrogen reduction of WO3-CuO powder mixtures

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## Abstract

Tungsten (W) is regarded as one of the prospective materials for the ultimate environment due to its excellent high-thermal properties such as high strength, high melting point, and low thermal coefficient. Meanwhile, W-Cu composite is appreciated as the desirable material for electric contact and arcing-resistant electrodes owing to its combined properties such as high strength and arc-resistivity from W and excellent thermal and electrical conductivity from Cu. However, it is difficult to fabricate the homogeneous W-Cu composites because of the mutual insolubility between W and Cu, the high melting point of W. Also, it is required to minimize impurities for giving good electrical conductivity. On the other hand, ball-milling route is one of the ways to fabricate homogeneous W-Cu composite powder, but there are serious drawbacks such as the contamination from milling media and the formation of hard aggregates during the milling process. Recently, a novel method, high-energy ball milling using metal oxide powder and hydrogen reduction, is reported for minimizing impurities and preventing the formation of aggregates. However, in order to satisfy the required properties, a systematic study on the dependence of powder purity and microstructure according to milling and hydrogen-reduction conditions is required. Therefore, this work focuses on the synthesis of homogeneous W-Cu composite powder with controlled properties by high-energy ball milling and hydrogen reduction of WO3 and CuO. Also, the optimal synthesis conditions of W-Cu composite powder are suggested, based on the observed microstructural charcteristics.

**Keywords:** WO3-CuO powder mixture, milling condition, hydrogen reduction, W-Cu powder

# POSTER Session 2

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| P-D0221 |

# Effects of zinc addition on deformation behavior of magnesium single crystals

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## Abstract

[11"2" $\bar{0}$] tensile tests of Mg-(0.16-0.27at. %) Zn single crystals with 3mm in width, 20mm in length and 0.3 mm in thickness were carried out to investigate the effect of Zn on the deformation of Mg. Second order <c+a> pyramidal slip (SPCS) was activated at yielding below room temperature (77K, 203K and 293K) in the Mg-Zn single crystals, similar to pure Mg. {10"1" $\bar{1}$} twinning occurred after yielding. In addition, first order pyramidal <c+a> slip (FPCS) was also activated at 77 K and 203 K. In the [11"2" $\bar{0}$] tensile test of pure Mg single crystals, yield stress increased with increasing temperature below room temperature, i.e., positive temperature dependence was observed. The yield stress at 77K-203K drastically increased by Zn addition and showed negative temperature dependence in the Mg-Zn alloys. CRSS for {10"1" $\bar{1}$} twins decreased by Zn addition. However, the tensile ductility of Mg single crystals scarcely increased by Zn addition.

**Keywords:** pyramidal slip, {10"1" $\bar{1}$} twin, yield stress, CRSS, ductility

# Fatigue fracture behavior of aluminum foils

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## Abstract

Fatigue properties of commercially pure aluminum (1N30 and 1085) and Al-Mn alloy (3003) foils with a thickness of 15 μm were investigated. The aluminum foils had elongated grains parallel to the rolling direction. Also, the fraction of low-angle grain boundary was higher than that of high-angle grain boundary. Fatigue strength at 107 cycles became greater in the following order, 1N30, 1085, and 3003. The order was in agreement with that of 0.2% proof stress. Fatigue limit was not observed until 107 cycles in the foils as well. The slope of S-N plots of 3003 was smaller than those of 1N30 and 1085, suggesting that fatigue lives of 3003 have more sensitive to stress amplitude. The relationship between the ratio of stress amplitude to 0.2% proof stress, σa/σ0.2, and the number of cycles was also investigated. The σa/σ0.2 at 107 cycles was the highest in 1085 and the lowest in 1N30. Chisel-edge like failures mainly occupied fracture surfaces in the all foils after fatigue tests. Commercially pure aluminum foils were suggested to have longer fatigue lives between crack initiation and failure, compared to 3003 foils.

**Keywords:** Al-Mn, 0.2% proof stress, chisel-edge, S-N plot

| P-D0224 |

# Effect of yttrium addition on bending deformation behavior of magnesium single crystal

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## Abstract

Yttrium addition to magnesium has been studied to improve the tensile properties. In this study, to investigate the effect of yttrium on the bending deformation behaviour of magnesium, three-point bending tests of rolled pure magnesium and Mg-(0.2~0.9)at.% Y alloys, were performed. Bending yield stress increased with yttrium addition. Bending ductility also increased with yttrium addition due to activation of non-basal slips. Bending ductility of specimen TR, whose rolled surface and neutral plane are parallel, increased with yttrium addition, while bending ductility of specimen TN, whose rolled surface and neutral plane are perpendicular, peaked at 0.5at.%Y.

To investigate the cause of the crystallographic orientation dependence of the bending deformation of rolled specimens, three-point bending tests of Mg-(0.23~0.68)at.%Y alloy single crystals were performed. Specimen B whose basal plane and neutral plane are parallel, corresponding to Specimen TR, and specimen E whose basal plane and neutral plane are perpendicular, corresponding to specimen TN were prepared. Both specimens showed an increase in bending yield stress with yttrium addition. Due to the increase in CRSSs of basal slip and {10"1" $\bar{2}$} twin by yttrium addition of 0.68 at.% Y suppressed {10"1" $\bar{1}$}-{10"1" $\bar{2}$} double twin, which is crack initiation site in magnesium, resulting in increased bending ductility of specimen E.

**Keywords:** {10"1" $\bar{2}$} twin, {10"1" $\bar{1}$}-{10"1" $\bar{2}$} double twin, basal slip, non-basal slip

Poster Session 2

| P-D0263 |

# Control of Ears on Aluminum Cup with Clad Sheet

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## Abstract

The deep drawing process makes it possible to form containers with seamless bottoms. Industrial products include those for automobiles and chemical plants. In order to enhance functionality, lightweight and high-strength containers are being formed. Aluminum, a representative light metal, has long been widely used in industrial products. Its thermal conductivity is three times that of iron, so it is used in various heat exchangers and heat sinks. In the deep drawing process, however, in-plane anisotropy causes ears to form on the edges of the drawn cup. Material loss becomes a problem due to the formation of ears at the opening of the drawn cup. Therefore, when deep drawing is performed with two blanks stacked on top of each other, the way the blanks are stacked affects the generation of ears on the drawn cup. In other words, when the direction of ear generation and the direction of no ear generation overlap in the two blanks, ear generation in the drawn cup would be suppressed. In the present study, deep drawing was performed with two blanks stacked on top of each other to suppress ear formation. To improve the bonding of the blanks, the laminated sheet was also fabricated using a resin sheet. When the two blanks were stacked, ear formation could be suppressed depending on the stacking method. Ear formation was also effectively suppressed in the forming of the laminated sheet.

**Keywords:** deep drawing, formability, earing formation, pure aluminium, thermoplastic resin

| P-D0461 |

# Effect of Mn and Mo addition and solution heat treatment on microstructure and hardness of Al-7Si-0.5Cu-0.5Mg alloy

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## Abstract

In order to improve mechanical properties of Al-7Si-0.5Cu-0.5Mg cast alloy, Mn and Mo were added in the alloy and their microstructure and hardness changes were investigated at different solution heat treatment temperatures. Al-Si-Cu-Mg-(Mn-Mo) alloys were cast into a permanent mold. The cast alloys were machined and solution heat-treated at the temperature range from 495 to 545°C for 5 hours, followed by water quenching. Microstructure of as-cast and heat-treated alloys were observed using the field-emission scanning electron microscopy. Brinell hardness test was conducted to evaluate the hardness values under the various alloy compositions and heat treatment conditions. In the case of Al-Si-Cu-Mg alloys without Mn and Mo contents, intermetallic phases including Q-Al5Cu2Mg8Si6, β-Al5FeSi, π-Al8FeMg3Si, θ-Al2Cu, and Mg2Si were identified in as-cast condition. When Mn and Mo content were added in the alloy, α-Al(Mn,Fe,Mo)Si phase was found instead of the β-Al5FeSi phase. When Mn and Mo were added in the Al-Si-Cu-Mg alloy, hardness of the alloy increased regardless of solution heat treatment temperatures. As the solution heat treatment temperature increased, hardness of the present alloys also increased. From the experimental results, effect of microstructure on hardness of Al-Si-Cu-Mg alloy was discussed.

**Keywords:** Aluminium alloy; microstructure analysis; transition metal; Brinell hardness; solution heat treatment

| P-D0529 |

# Effect of Cu addition on the kinetics of cluster formation in Al-Mg-Si alloys

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## Abstract

Fuel efficiency and exhaust gas regulations for automobiles are becoming increasingly stringent. Aluminum, with its excellent strength-to-weight ratio, allows for lightweighting and has been the subject of extensive research. The addition of Cu in Al-Mg-Si alloys is known to have a significant impact on the microstructure and mechanical properties. However, the kinetics of cluster formation is not fully understood. In this study, we analyzed the influence of Cu addition on the kinetics of cluster formation in Al-Mg-Si alloys using a differential scanning calorimeter(DSC). The peak for cluster was confirmed. And two types of nanocluster were analyzed through the peak separation using Gaussian method from the overlapped peak based on. The activation energy was obtained based on DSC measurement. Moreover, the mechanical property using micro Vickers hardness is also affected by Cu addition. The clustering behavior is discussed based on the age-hardening behavior.

**Keywords:** Al-Mg-Si Alloy, Cu addition, cluster formation, DSC, precipitation formation, thermal behavior

| P-D0530 |

# Effection of Sn addition of Age-hardening behavior in Al-Mg-Si alloys

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## Abstract

Aluminum alloys have been developed for better efficiency and stability due to severe environmental regulations. 6xxx (Al-Mg-Si) alloys are widely used for automobile frames because it has high strength, corrosion resistance and heat resistance. However, in the process of transporting and storing in aluminium sheet, it is inevitably exposed at room temperature and undergoes natural aging (NA). Due to the formation of clusters during the natural aging, the strength is reduced by suppressing the formation of the main strengthening phase generated during age hardening. Pre-aging (PA) treatment is performed in order to suppress such a decrease in strength.

In this study, we investigate changes in mechanical properties and aging behavior of Al-Mg-Si and Al-Mg-Si-Sn alloys using Vickers hardness and Differential Scanning Calorimetry (DSC) and Transmission Electron Microscope (TEM). Three heat treatment methods: Single aging (SA), Two-step aging (NA-AA), Multi-step aging (PA-NA- AA), were conducted to understand effect of Sn addition on the age hardening behavior

**Keywords:** Al-Mg-Si alloys, Sn addition, Natural aging, Pre-aging, Age hardening behavior

Poster Session 2

| P-D0553 |

# Effect of cold-rolling on aging behaviour of Al-Cu-Mg alloy at different aging temperatures

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## Abstract

Al-Cu-Mg alloys are known as 2xxx series aluminium alloys which is represented by the duralumin and super duralumin, and it is widely used in aerospace and transportation industries due to its excellent mechanical properties. Al-Cu-Mg alloys have been studied conventionally as age-hardening alloys. It has been reported that mechanical properties of Al-Cu-Mg alloys can be enhanced by introducing cold-rolling before aging.

The precipitation sequence for Al-Cu-Mg alloys is generally described as followed as: S.S.S.S.→ G.P. Zone→ metastable θ' phase→ stable θ phase or S.S.S.S.→ G.P.B. Zone→ metastable S' phase → stable S phase. The precipitation sequence of this alloy series is related with the Cu/Mg ratio. It has also been reported that the Ω-phase precipitates in Al-Cu-Mg-Ag alloys. Ω-phase precipitates on slip plane of Al matrix. Therefore, it is believed to contribute to the improvement of mechanical properties It also exhibits good thermal stability and is resistant coarsening. Furthermore, it has been confirmed that the Ω-phase precipitates the alloy that does not contain silver with a specific Cu/Mg ratio by aging treatment of cold-rolled alloys.

The purpose of this research is to investigate the effect of aging treatment temperatures of 423K, 473K, and 523K on the Ω-phase precipitation in cold-rolled alloys.

**Keywords:** Al-Cu-Mg alloy, aging, cold-rolling, precipitation, TEM

| P-D0554 |

# Microstructure observation of Al-1.0mass%$Mg_2Si$ alloy added Cu, and Ni

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Al-Mg-Si alloys (6xxx Al alloy series) are one of the age-hardenable aluminum alloys. The precipitation sequence is as follows: super saturated solid solution (SSSS) → cluster/GP zones → needle-like β" / parallelogram shaped precipitates → rod-shape β' → type A/B/C precipitates → plate-like β (Mg2Si) precipitates. Al-Mg-Si alloys have high strength-to-weight ratio, high ductility, good extrusion formability and good corrosion resistance by anodic oxidation treatment. Since Al-Mg-Si alloys are medium-strength, various additives have been used to increase their strength. The purpose of this study is to investigate the effects of additive elements (Cu, Ni) on the microstructure of Al-Mg-Si alloys. (1) Al-1.0mass%Mg2Si, (2) Al-1.0%Mg2Si-0.5%Cu (mass%), and (3) Al-1.0%Mg2Si-0.2%Ni (mass%) were fabricated. Micro-Vickers hardness tester and transmission electron microscope (TEM) (120 kV) were used to investigate the microstructural changes of each alloy. Vickers hardness tester showed that the added elements were harder than Base alloy. TER observation from the [100]Al direction showed that the number density increased, and precipitate length decreased in the alloys with Cu and Ni added compared to the Base alloy, indicating that the added elements precipitate finer. Rod-shaped precipitates of needle-like β" / parallelogram-type precipitates growing in the direction and their cross sections were observed in all alloys. Q' (Cu-containing precipitate) and its precursors were also observed in the Cu-doped alloys.

**Keywords:** Al-Mg-Si alloy, aging, Cu-addition, precipitation, TEM

| P-D0588 |

# Effects of homogenization and Mn addition on the mechanical properties of Fe-containing Al-Mg-Si alloys

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## Abstract

Al-Mg-Si alloys are widely used for construction components such as window frames since they have good balance between strength and ductile and extrudability. Suitable alloying elements i.e. Mg, Si and Fe are required to decrease energy expenditure, improve extrudability during extrusion. Fe contents give rise to the formation of platelet Fe-intermetallic compounds (Fe-IMCs) during casting. They are harmful for extrudability and ductility. Thus, controlling the detrimental Fe-IMCs is a key point to make excellent extrudability of billets and high quality of properties.

In this study, different homogenization treatments and Mn addition were conducted to understand the phase transformation of Fe-IMCs and to investigate relationship between microstructure and mechanical properties of high Fe-containing Al-Mg-Si alloys. Size and area fraction of Fe-IMCs were quantitatively evaluated after dual rate cooling (DRC).

**Keywords:** homogenization, Mn addition, dual rate cooling, Fe-intermetallic compounds, elongation, extrudability.

| P-D0591 |

# Static recrystallization behavior of laser shock peened AZ31 Mg rolled sheet

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## Abstract

Magnesium alloys exhibit poor mechanical properties and limited formability at room temperature due to their anisotropic hexagonal close-packed (HCP) structure and lack of independent slip systems. To overcome these limitations, texture weakening has emerged as a highly effective approach. Among the various methods available, Laser Shock Peening (LSP) has been recognized as a promising technique for weakening the texture through deformation twinning. LSP is a non-thermal surface treatment process that involves the generation of rapid expansion of high-temperature and pressure plasma using a laser beam. This process induces extremely high stresses exceeding 1 GPa in localized areas, resulting in the development of strong compressive residual stresses and plastic deformation on the material surface. LSP treatment enhances the overall mechanical performance of Mg alloys by improving their ability to accommodate plasticity through the promotion of deformation twinning. In this study, our objective is to investigate the static recrystallization behavior of Mg rolled sheets treated with LSP in order to enhance their mechanical properties. The microstructure was identified using OM and EBSD, and static recrystallization behavior was investigated by analyzing the fraction of deformation twinning and intensity of texture using OIM software. The microstructure analysis, including the examination of the fraction of deformation twinning and the intensity of texture, was carried out using Optical Microscopy and Electron Backscatter Diffraction techniques. These methods were employed to gain a deeper understanding of the static recrystallization behavior in the LSP-treated Mg rolled sheets.

**Keywords:** magnesium alloy, laser induced shock peening, heat-treatment, texture, deformation twin

| P-D0646 |

# Effect of Mechanical Properties by Addition of Rear Earth Elements in Al-SI-Mg Alloy using Machine-Learning Models

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## Abstract

Al-Si-Mg-based aluminum alloys are widely used as lightweight materials due to their excellent castability, mechanical properties and wear resistance. Recently, studies to improve mechanical properties according to microstructure changes by adding rare earth elements have been reported. In this study, the changes in mechanical properties of Al-Si-Mg-based alloys were observed according to the addition of lanthanum (La) among rare earth elements, and an alloy design was optimized using machine-learning models. Aluminum alloys were produced by gravity casting and die casting with different addition amounts of La elements. The mechanical properties and microstructure of the alloys were analyzed using Vickers hardness test, tensile test and FE-SEM/EDS. For machine-learning, experimentally produced aluminum alloy properties and values extracted from previous papers were used. The collected data was learned through an several machine-learning algorithms. we tried to predict the optimal amount of La addition for improve mechanical properties.

**Keywords:** Al-Si-Mg alloy, machine-learning, mechanical properties, rear earth elements

| P-D0648 |

# Evaluation of microstructure and mechanical properties of ultralight Mg-Li alloys

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## Abstract

Magnesium alloy is the lightest structural material among commercial alloys and is widely used for electronic product cases such as laptops, PCs, and mobile phones due to its excellent specific strength and electromagnetic wave shielding properties compared to other lightweight materials. In addition, Mg-Li-based alloys with the addition of Li, an ultra-light metal element, are attracting much attention as materials for aerospace such as rockets and missiles because they can dramatically lower the density of conventional magnesium to increase specific strength. However, due to poor strength and formability at room temperature, application to actual parts is limited. Since the crystal structure of magnesium is a dense hexagonal (hcp) structure, the room temperature slip system required for plastic deformation is limited, resulting in low formability. In this study, magnesium alloys with different HCP and BCC phase fractions were prepared by adding 6, 8, and 10 wt.% of Li element to improve the formability of magnesium, and the microstructure, mechanical properties, and welding characteristics according to the phase fraction change. A study was conducted on Each magnesium alloy specimen was gravity cast in an SF6 + CO2 gas atmosphere using an electric furnace, and after homogenization at 350 °C for 4 hours, direct extrusion was performed at 200 °C to produce an extruded material having a thickness of 4 mm and a width of 50 mm. An optical microscope, SEM, etc. were used for microstructure and phase analysis, X-ray diffraction analysis was used for phase analysis, and argon welding was used to bond the samples according to the change in Li addition amount. Tensile tests were conducted at room temperature to evaluate the mechanical properties of extruded materials and welded samples.

**Keywords:** Magnesium, Lithium, Extrusion, Microstructure, Mechanical properties

| P-D0654 |

# Effect of aging conditions on hydrogen release behavior in fractured Al-Cu alloy in humid and dry environments

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## Abstract

High-strength aluminum alloys may lose ductility due to hydrogen embrittlement. In general, Al-Zn-Mg(-Cu) alloys tend to be embrittled because of potential differences around grain boundaries related to these alloy compositions. However, Al-Cu(-Mg) alloys have excellent hydrogen embrittlement resistance regardless of alloy composition and aging conditions. These findings can be applied to future material development if we can elucidate the hydrogen embrittlement mechanism and microstructural factors that improve susceptibility to hydrogen embrittlement. In this study, 2219 alloy, a commercial Al-Cu alloy, was solution-treated at 535°C for 1h and then aged under various conditions to investigate the effects of aging conditions on hydrogen release behavior in fractured specimens. The slow strain rate technique tensile test showed that aging at 100°C or 130°C after solution treatment resulted in higher strength and ductility than the conventional aging at 190°C. As for the effects of the test environment, 0.2% proof stress and ultimate tensile strength did not change, but elongation to failure decreased in some specimens in the humid environment. Thermal desorption gas chromatography of the fracture specimens showed that the original trapping sites differ depending on the aging conditions, and that the trapping sites and the amount of hydrogen released from them were affected by the test environment.

**Keywords:** Al-Cu, hydrogen embrittlement, grain boundary, slow strain rate technique, thermal desorption gas chromatography

| P-D0877 |

# Recrystallization behaviour and stretch formability of Mg-Al-Zn-Ca-Y alloy sheet

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## Abstract

In this talk, the effects of Al content on the texture evolution of Mg-xAl-1Zn-0.1Ca-0.2Y alloy sheets fabricated by hot rolling, cold rolling, and subsequent annealing processes will be addressed in detail. It was found that a smaller Al addition led to a larger amount of free Ca solute atoms being available to contribute to co-segregation with Zn, resulting in delayed recrystallization of the cold-rolled sheets during annealing and a change in the basal pole figure shape of the annealed sheets. A quadruple basal texture, in which the positions of the four peaks of the basal poles were developed at tilt angles of ±25° to the RD and ±40° to the TD from the normal direction (ND), was obtained in the annealed Mg sheets. A smaller amount of Al caused an increase in the intensity of the main peaks along the TD but a decrease in the intensity along the RD. As a result, the texture of the annealed sheets gradually changed from RD-split to diamond and TD-split in the (0002) pole figure, as shown by the relative comparison of pole intensities in the RD and TD. This texture change strongly affected the Schmid factor (SF) for basal slip. In the alloys investigated in this study with an off-basal texture, as the maximum intensity of the basal poles increased, the average SF of the basal planes also increased, making basal slip easier.

**Keywords:** Magnesium alloys, Stretch formability, Corrosion resistance, Recrystallization, Sheet

| P-D0905 |

# Effect of aging temperature on the precipitation behavior and mechanical properties of Al–Zn–Mg–Cu alloy

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## Abstract

We investigated the effect of aging temperature on the precipitation behavior and mechanical properties of Al–7.6Zn–2.7Mg–2.0Cu–0.1Zr–0.07Ti (wt.%) alloy utilizing microhardness, electrical resistivity, X-ray diffraction, differential scanning calorimetry (DSC), transmission electron microscopy (TEM), atom-probe tomography (APT), and tensile testing. At aging temperatures of 80–220 °C, the aging times to reach the peak hardness and the electrical resistivity values under the peak hardness condition decrease with increasing aging temperature. The type of nanoprecipitates formed under peak-aging conditions changes with aging temperature: coherent GPI zones at 80 °C, GPII zones with minor η' at 120–150 °C, and η'/η with minor GP zones at 180–220 °C. The GPI and GPII zones formed at 80–150 °C contain similar amounts of solute atoms, whereas the η'/η precipitates formed at 180 °C contain larger amounts of solute atoms. The strength of the peak-aged alloy decreased with increasing aging temperature due to increased size and decreased number density of the nanoprecipitate. Under peak-aging conditions, precipitation strengthening originate mainly from dislocation shear at 80–150 °C and Orowan bypass above 180 °C. The shearable to non-shearable transition of the nanoprecipitates at 180 °C reduces strain hardening, thus deteriorating the alloy ductility.

**Keywords:** aluminium alloys; precipitation; tensile properties; transmission electron microscopy; atom probe tomography

|P-D0943 |

# Effects of mechanical milling and post heat treatment on on the microstructure and mechanical properties of Al-Zn-Mg-Cu-Si alloys with and without Zr manufactured by spark plasma sintering

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## Abstract

7xxx Al-Zn-Mg-Cu alloys have been widely used in automotive industry because of their light-weight and excellent mechanical properties, which result from nano-sized precipitates formed during adequate solution and aging heat treatments. Silicon has been added to 7xxx alloys to modify nanoprecipitates and suppress casting defects such as hot cracking and tearing. Zirconium has been often added to 7xxx alloys for controlling the microstructure and improving mechanical properties due to precipitation strengthening and grain pinning effects of L12-Al¬3Zr nanoprecipitates. Powder metallurgy using mechanical milling and sintering is one of promising means to manufacture ultrafine-grained (UFG) Al alloys with excellent mechanical properties. The mechanical milling significantly affects the microstructure (e.g., dislocation density, grain size) and nanoprecipitates. The heat treatment is also an important process parameter controlling microstructure and nanoprecipitates. In this study, therefore, we investigated the effect of mechanical milling and post heat treatment on the microstructural evolution and mechanical properties of Al-Zn-Mg-Cu-Si alloys with and without Zr. The Al-Zn-Mg-Cu-Si alloys with and without Zr were manufactured by high energy ball milling (HEBM) and spark plasma sintering (SPS). The sintered alloys were heat-treated at 500 °C for various holding times. Micro- and nano-structures of powders and sintered alloys were observed using scanning and transmission electron microscopes and their effects on the mechanical properties were discussed.

**Keywords:** Al-Zn-Mg-Cu-Si alloy, Ultrafine grained alloy, Spark plasma sintering, Transmission electron microscopy

| P-D1061 |

# A Comprehensive Investigation into the Microstructural and Mechanical Response of Ti Alloys after Electrochemical Hydrogen Charging

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## Abstract

Ti alloys are mostly employed in a wide range of applications, especially for aviation and medical purposes, due to their high specific strength and outstanding corrosion, and mechanical properties. However, hydrides can easily form in the microstructures of Ti alloys due to the high reactivity of Ti element to hydrogen, which subsequently impacts their mechanical properties. The purpose of this study is to analyze the microstructure and mechanical properties of Ti alloy after electrochemical hydrogen charging. Hydrogen is initially charged into the microstructure of the Ti alloy by electrolysis. Afterward, the hydride formation in the microstructure with charging time is confirmed with an X-ray diffractometer. The hardness values are measured along the depth direction from the surface to figure out the degree of penetration of hydrogen. Based on them, microstructural evolution with the charging time is analyzed with Electron BackScatter Diffraction (EBSD) microscope. In addition, compression test is conducted to evaluate the mechanical strength of hydrogen-charged Ti alloys.

**Keywords:** Ti alloys, hydrogen embrittlement, electrochemical hydrogen charging, mechanical properties, microstructure

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| P-E0267 |

# A multi-phase-field framework for predicting material microstructures formed by different scanning patterns in powder bed fusion

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## Abstract

Metal additive manufacturing (AM) can fabricate material parts that have complex shapes. Recently, by controlling the scanning strategy, it has become possible to control not only the shape of parts but also the material microstructures. For example, Naresh et al. investigated the impact of four different scanning strategies on the microstructures developed during powder bed fusion (PBF) of the Inconel 718 alloy [Addit. Manuf. 38 (2021) 101792]. However, because the number of possible combinations of scanning parameters is vast in PBF-AM, the use of numerical simulations for microstructures prediction has become essential. Cellular automaton has been widely used to predict microstructures, although its computational accuracy is a concern. The phase-field (PF) method is the most accurate approach that can be used to predict mesoscale microstructures. Chadwick and Voorhees succeeded in representing grain growth during PBF-AM using the multi-phase-field (MPF) method with Rosenthal equation [Acta Mater. 211 (2021) 116862]. We applied this method to PBF-AM with multi-layer and multi-track scanning and expressed epitaxial grain growth [Mater. Trans. (2023) in press]. However, because of the high computational costs, simulations have been limited to low laser power. In this study, we developed an efficient MPF simulation framework, in which the computational domain was limited to the area around the melt pool, to enable a systematic evaluation of microstructures obtained using different scanning strategies.

**Keywords:** Phase-field simulation; Large-scale computation; Powder bed fusion; additive manufacturing; Material microstructure.

| P-E0367 |

# Melting and Solidification of Stainless Steels Induced by Laser-Beam Irradiation for Powder Bed Fusion Process

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## Abstract

According to the generally accepted Hunt's columnar-to-equiaxed transition (CET) criterion, a higher temperature gradient (G) at the solidification front is preferable to a lower one for columnar grain formation [J.D.D. Hunt, Mater. Sci. Eng., 65 (1984) 75]. We have previously performed electron beam irradiation experiments and simulations of 304 and 316L stainless steels and examined the relationship between the microstructure formed and the solidification conditions, and found a trend opposite to the CET criterion, suggesting equiaxed grain formation due to high-velocity flow [Y. Miyata, M. Okugawa, Y. Koizumi, T. Nakano, Crystals, 11 (2021) 856]. In this study, laser irradiation experiments were conducted on five types of stainless steels with different liquidus-solidus temperature differences (ΔT0) and carbon contents to elucidate the dominant factors in the formation of solidification microstructures in laser beam powder bed fusion. The cross-sectional shapes of the formed melt-regions and microstructures were analyzed by field emission scanning electron microscopy and backscattered electron diffraction analysis. Computational thermal-fluid dynamics simulation with absorption coefficient adjusted as a fitting parameter reproduced the experimentally observed shape of the melt-region, and the G and R at the solid-liquid interface were evaluated and their relationship with the microstructure was investigated. Under the solidification conditions, both the G and R were large, and the microstructures have a trend opposite to that of the CET criterion, suggesting the influence of equiaxed grain formation due to high-velocity flow even in LB-PBF. The microstructure formed by laser irradiation tended to become more equiaxed with decreasing ΔT0 and carbon concentration.

**Keywords:** Additive manufacturing, Stainless steel, columnar-to-equiaxed transition, CtFD simulation

| P-E0681 |

# Study on the Microstructure, Mechanical Properties and Electrical Conductivity of Al-Si-Mg Powder by PBF process according to Si and Mg Content Change and Heat Treatment Conditions

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## Abstract

Aluminum alloys are considered promising materials for the automotive and aerospace industries due to high specific strength, thermal conductivity, and low density. They have the potential to replace copper alloys in various applications. In this study, we investigated the enhancement of microstructure, mechanical properties, and thermal properties through variations in Si and Mg content and heat treatment conditions (none, 250°C 2h, 350°C 2h, 450°C 2h).

The aluminum alloy powders were manufactured through the gas atomization process. Specimens were produced using the powder bed fusion technique. The PBF process was conducted with laser power, hatch size, and speed (290W, 0.08mm, 800mm/s).

The microstructure was observed using a FE-SEM under various heat treatment conditions. SEM images revealed different microstructures for each heat treatment condition. Precipitation of Si was observed at 350°C, and further coarsening occurred at 450°C. For mechanical property evaluation, measurements were performed using a Vickers hardness tester. The Vickers hardness results showed a decrease in hardness values (128, 115, 104, 100, 98 Hv) with decreasing wt% of Si and Mg. Furthermore, the hardness value decreased to 128, 111, 78, and 46 Hv when heat treatment was performed on the Al-10Si-0.5Mg alloy. To evaluate thermal properties, electrical conductivity measurements were conducted using an electrical conductivity meter. The electrical conductivity results demonstrated an increase in conductivity (22, 23, 24, 27, 29%IACS) with decreasing wt% of Si and Mg. The thermal conductivity value predicted by electrical conductivity improved to 96, 166, 175, 179 W/mK when heat treatment was applied to the Al-10Si-0.5Mg alloy.

**Keywords:** aluminum, 3D printing, microstructure, mechanical properties, thermal properties

| P-E0701 |

# The Gibson-Ashby model for additively manufactured metal lattice materials: Its theoretical basis, limitations and new insights from remedies

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## Abstract

The Gibson-Ashby (G-A) model has been instrumental in the design of additively manufactured (AM-ed) metal lattice materials or mechanical metamaterials. The first part of this work reviews the proposition and formulation of the G-A model and emphasizes that the G-A model is only applicable to low-density lattice materials with strut length-to-diameter ratios greater than 5. The second part evaluates the applicability of the G-A model to AM-ed metal lattice materials and reveals the fundamental disconnections between them. The third part assesses the deformation mechanisms of AM-ed metal lattices in relation to their strut length-to-diameter ratios and identifies that AM-ed metal lattices deform by concurrent bending, stretching, and shear, rather than just stretching or bending considered by the G-A model. Consequently, mechanical property models coupling stretching, bending and shear deformation mechanisms are developed for various lattice materials, which show high congruence with experimental data. The last part discusses new insights obtained from these remedies into the design of strong and stiff metal lattices. In particular, the use of inclined struts should be avoided.

**Keywords:** Additive manufacturing, Metal lattice, Strength, Elastic modulus, Topology design, Mechanical metamaterials

| P-E0743 |

# Characterization of flowability in gas-atomized Inconel 625 powder for additive manufacturing applications

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## Abstract

Additive manufacturing (AM) techniques have gained increasing attention in recent years to produce different metals and alloys. The quality of additive manufactured components depends on the flowability of the feedstock powders. Therefore, a comprehensive understanding of flowability and characteristics of powders is imperative in developing of AM processes. In this study, spherical and fine Inconel 625 powders with homogeneous distribution was produced by gas atomization, and the flowability of particles was systematically investigated in terms of particle size distribution (PSD). Despite requiring a higher avalanche energy of 9 mJ/kg, powders with a uniform PSD of 50-100 mm with a sphericity value of 0.90 had the highest flowability. On the other hand, powders with a PSD of 50-150 μm and a sphericity value of 0.71 showed lower flowability and an avalanche energy of 6 mJ/kg. The hardness of the powders with the narrowest PSD was measured to be 304 HV, which was higher than those of the coarse size distributed (297 HV) and mix size distributed (289 HV) powders. The Hall velocity of 14.5 s/50g in large particles was attributed to their greater mass and inter-particle bonds, which made them more resistant to the forces that cause particles to separate. The findings indicated that particle size distribution is a critical factor in achieving optimal flowability and powder characteristics, which has important implications for the additive manufacturing of Inconel 625.

**Keywords:** Inconel 625 powder, Additive manufacturing, Gas atomization, Flowability, Microstructure evaluation.

| P-E0748 |

# Effect of single melt pool shape on relative density and mechanical properties of additively manufactured Inconel 625 alloy

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## Abstract

In Laser Powder-bed Fusion process, Input laser power and scanning speed are important parameters to control the shape of single melt pool which determine the relative density and surface roughness of final products. Understanding the relationship between single melt pool formation phenomenon and relative density with varied process parameters allows less experiment time and clarified for the industrial applications. In this study, the relative density and mechanical properties of the additively manufactured Inconel 625 alloy are consequently evaluated compare to the varied input power and scan speed parameters.

**Keywords:** Additive manufacturing, super alloy, Melt pool, density

| P-E0774 |

# Geometric characteristics in polycaprolactone (PCL) scaffolds produced by materials extrusion-based additive manufacturing

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## Abstract

Materials extrusion-based additive manufacturing is known as a promising technique to fabricate the scaffolds due to affordability, versatility, and wide acceptance of various materials. The reliability and controllability of the printing process are necessary to produce scaffolds with desired properties for tissue engineering. Analytical models are developed in this study to simulate the geometric characteristics of cylindrical polycaprolactone (PCL) scaffolds produced by the materials extrusion-based additive manufacturing technique using fluid mechanics. The geometric characteristics of the PCL scaffold can be predicted by using extrusion pressure, temperature, nozzle diameter, nozzle length, and printing speed. The effectiveness of models is verified through comparison with the experimental results. Simulation results show that geometric characteristics have a strong relationship with processing parameters, and the developed models are useful in predicting the geometric characteristics of the scaffold structure produced by the materials extrusion-based additive manufacturing technique.

**Keywords:** Additive manufacturing; Polycaprolactone; Scaffold; 3D bioprinting; Porosity

| P-E0783 |

# Wire-fed Additive Manufacturing of Cu and Cu-based Alloys for Application in the Spent Nuclear Fuel Canister

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## Abstract

The spent nuclear fuels are confined in a storage canister and disposed underground until the fuels are exhausted. The outer most material of the canister is oxygen-free Cu because of its prominent corrosion-resistance in a deep geological environment. KAERI is developing the new material as well as new manufacturing process for the corrosion-resistant layer. Cu and Cu-based alloys was formed using wire-fed AM and powder-fed AM. Wire feeding was much faster than powder feeding to form a certain thickness of cladding layer. Moreover, the developed wire feeding AM was advantageous in material saving and production delivery in comparison to a conventional forming process of sheathing. Both the microstructures and the corrosion resistance of the cladded layer were investigated to ensure the prolonged storage circumstances. The Cu and Cu-based alloys formed on steel substrates were strikingly dense without any pores and revealed diffusion bonding structures. Depending on the alloys the grain morphologies were varied from equiaxed to elongated. The correlation between the microstructures and the alloying elements will be discussed.

**Keywords:** Additive Manufacturing; Direct Energy Deposition; Wire; Cladding; Cu alloy

| P-E0884 |

# Carbon Nitride (C3N4) as a Filler of Epoxy-Acrylate based Resin for the Digital Light Processing (DLP) 3D Printing Process

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## Abstract

3D printing offers extensive design flexibility for producing complexed-shaped products that were previously unattainable using conventional manufacturing methods. The polymer industry, which demands the fabrication of intricate structures, has been actively exploring various polymer 3D printing techniques such as fused deposition modeling (FDM), selective laser sintering (SLS), stereolithography (SLA), and digital light processing (DLP). Among these methods, DLP 3D printing, which is a widely adopted photocuring 3D printing technique, stands out for its rapid printing speed with each layer solidified and laminated with a planar light source. This process presents exceptional precision and surface quality. However, DLP 3D printing faces a limitation in terms of the mechanical strength of its product due to inherent characteristics of photocurable resins, such as low crosslinking density and challenges in controlling the optimal curing irradiation time and anisotropy during the 3D printing process. In this study, we presented a novel approach to enhance the strength of DLP products by utilizing graphitic carbon nitride (g-C3N4) as a filler for standard DLP acrylic resin. g-C3N4 has multiple hydrogen bonding motifs (-NH2, -NH functional groups) in the molecule, which could induce hydrogen bonding between matrix and g-C3N4, thereby increasing the intermolecular interaction, and resulting in improved mechanical properties. Our investigation focused on examining the filler characteristics of g-C3N4 and optimizing the DLP composite production process. The results confirm a significant increase in the tensile strength (22%) and the elastic modulus (34%) of the DLP output when utilizing composite material compared to the neat DLP polymer specimen.

**Keywords:** 3D printing, Digital Light Processing (DLP), Filler, g-C3N4

| P-E0889 |

# Lignin Reinforced Photo-curable Resin for Digital Light Processing

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## Abstract

Lignin which is a major component of the lignocellulosic matrix constitutes approximately 20-35% of the woody biomass. Lignin plays a crucial role in enhancing the strength and durability of wood, along with possessing bio-adhesive properties that make it suitable for biomedical materials and applications. Moreover, it is considered that lignin is a cost-effective renewable resource, contributing to reducing environmental issues in various industries such as forestry, chemical, and energy. Among the 3D printing technologies, DLP 3D printing, which implements 3D structures with photo-curable materials by selective light source irradiation, has great attention as a promising manufacturing process due to excellent surface quality with high throughput. Although DLP 3D printing has these advantages, its feedstock is limited to only photo-curable epoxy-acrylate (EA) resin, and the mechanical properties of DLP products with photo-curable feedstock are far away from the industrial demands. In this study, we introduce lignin as a reinforcement with photo-curable EA resin for DLP 3D printing. Lignin has many adaptable functional groups such as hydroxyl which could improve mechanical properties by interaction with acrylate matrix molecules. We optimized the dispersion processes (Magnetic Stirrer, Planetary Mixer, Ultra Sonicator) to uniformly disperse the lignin powder in EA resin, and printed out the DLP specimens to evaluate the effect of lignin molecules on the improvement of mechanical properties. It is demonstrated that the lignin-EA composite specimens demonstrate increments in tensile strength (42%) and hardness (21%) compared to those of neat EA resin specimens.

**Keywords:** Lignin, Biomass, Digital Light Processing(DLP), Composite, Mechanical properties

| P-E0890 |

# The New Approach for Developing ZrO2 Feedstock for Materials Extrusion 3D Printing

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## Abstract

Ceramics, which have excellent strength and hardness, high heat and chemical resistance, and unique photoelectric properties are widely applied as critical materials in various industries such as machinery, electrical device, and medicine. Ceramic feedstock in the form of slurries has been great attention for implementing intricate and sophisticated structured products. Accordingly, many attempts have been made to produce parts with complex and precise shapes by using ceramic slurry to 3D printing technology. In the 3D printing process with the use of ceramic feedstock, inkjet printing, and material extrusion methods are commonly used. However, there are limitations to the wide use of 3D printing technology with ceramic feedstock due to difficulties in the dispersion of ceramic powder in a feedstock and regulating its rheology enough to retain 3D printed shape during the printing process. In this study, we suggest a new approach to develop a ceramic (ZrO2) feedstock for slurry-based ceramic 3D printing to overcome the limitations by using polyethylene glycol (PEG) in diverse molecular weight (M.W. 400 – 8,000,000). A high ceramic content of 82.22% could be achieved for material extrusion 3D printing. Also, the rheology of ZrO2 feedstock can be varied by the selection of the molecular weights and combination of two or more different molecular weights of PEG. This study presents a novel method of developing ceramic feedstock for advanced ceramic 3D printing technology.

**Keywords:** Ceramic slurry 3D printing, Additive manufacture, zirconia, Polyethylene glycol

| P-E0951 |

# Mechanical responses of 304L stainless steel additively manufactured by laser powder bed fusion at 4.2K

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## Abstract

In this study, the extremely low temperature mechanical properties down to liquid helium temperature (4.2K) of 304L stainless steel additively manufactured by laser powder bed fusion (LPBF) were investigated. Initial microstructure revealed that the LPBF 304L stainless steel exhibited hetero-structured grain morphologies with a single face-centered cubic structure. Moreover, dislocation induced cell structures and in-situ nano oxides were observed within the grains. Compared to the wrought counterpart, the present alloy showed relatively higher yield- and tensile-strengths from room temperature down to liquid helium temperature. On the other hands, the present alloy experiences highly serrated flow, known as discontinuous plastic flow, leading to sudden failure. Based on the correlations between microstructural evolution and mechanical responses at liquid helium temperature, the deformation mechanisms were systematically discussed.

**Keywords:** 3D Printing, Laser Powder Bed fusion, Liquid helium, Cryogenic, Tensile properties, microstructure

| P-E0994 |

# Microstructure and magnetic properties of Fe-Ni alloy fabricated by Laser powder bed fusion process

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## Abstract

This study investigated microstructure and magnetic properties of Fe-45%Ni (wt%) alloy fabricated by the laser powder bed fusion process. The influence of processing parameters on microstructure and defect formation were studied in as-built condition using optical microscopy (OM) and scanning electron microscope (SEM). The results show that the processing parameters with laser power of 85W, scan speed of 300mm/s, hatching space of 0.105mm were optimized condition for a formation of high relative density (97.7%) and low defects. The crystallographic structure and orientations of the best specimens were determined by electron-backscatter diffraction (EBSD) analysis. Tensile specimens and toroidal cores were additionally fabricated using the optimized processing parameters. In order to reduce residual stress and form an appropriate microstructure, the effect of the post-heat treatment process according to temperature and time parameters was further studied. The tensile and magnetic properties of as-built and heat-treated specimen were measured. This study provides a well-defined processing conditions and mechanical/ magnetic properties of Fe-Ni alloy prepared by laser powder bed fusion process

**Keywords:** Fe-Ni alloy, Powder bed fusion, post-heat treatment, tensile properties, Magnetic properties, Additive manufacturing

| P-E1116 |

# Cryogenic tensile behavior of carbon-doped CoCrFeMnNi high-entropy alloys additively manufactured by laser powder bed fusion

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## ABSTRACT

High-entropy alloys (HEAs) having no single dominant element in contrast to conventional alloys, substantially increases the possibility of the discovery of new alloys via traditionally uncommon element grouping. Among them, the HEAs having a single face-centered cubic (FCC) structure (typically, Cantor alloy: CoCrFeMnNi) have been extensively studied due to their outstanding mechanical performance at the cryogenic temperature. However, FCC-structured HEAs often exhibit a critical drawback: insufficient yield strength, while their ductility is superfluous. To overcome these drawbacks, it was suggested that the addition of carbon to FCC-structured HEAs could enhance the mechanical properties via solid solution strengthening and precipitation hardening. Recently, it has been reported that additive manufacturing (AM) has great potential to obtain not only a high degree of design freedom of product shape but also superior mechanical properties of the HEAs. Recent studies reported that AM techniques could offer the dramatic enhancement of mechanical properties of the FCC-structured HEAs via generating a hierarchical heterogeneous microstructure. Meanwhile, although the cryogenic mechanical properties of the HEAs is a key issue for the HEAs and AM communities, there are few studies for the cryogenic mechanical behavior of the additively manufactured HEAs. In this study, we investigated the cryogenic mechanical behavior of carbon-doped CoCrFeMnNi alloy fabricated by laser powder bed fusion (L-PBF) that is the most famous AM technique. As a result of study, the significant enhancement of both strength and ductility of the L-PBFed alloy at the cryogenic temperature was confirmed, and the relationship between microstructure and mechanical properties were systematically investigated with a discussion of cryogenic deformation behaviors of the alloy.

**Keywords:** High-entropy alloy, laser powder bed fusion, Microstructure, Tensile properties, Cryogenic temperature

| P-E1118 |

# Effect of Substrate Pre-heating on Microstructure and Magnetic Properties of Nd-Fe-B Permanent Magnet Manufactured by L-PBF

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## Abstract

Since Nd-Fe-B permanent magnet has been attracting considerable attention due to its superior magnetic properties, this material is widely demanded used in various high-tech industries such as automobile and electronic applications. However, because the low formability of Nd-Fe-B magnet due to its brittleness, the freedom of shape design for improving performance of magnet is still limited based on traditional manufacturing techniques. Recently, the emergence of additive manufacturing (AM) technologies, known as 3D printing, allows irreplaceable advantage in fabrication of 3D product with near-net shape, surpassing traditional fabrication methods. Among the various AM techniques, laser powder bed fusion (L-PBF) stands out as one of the most popular methods, which offers significant design freedom making it particularly suitable for production of geometrically-complex parts. Therefore, the recent studies have intensively focused on applying L-PBF process to Nd-Fe-B magnet for overcoming the limitation of design freedom of the magnet used in high-tech applications such as high-efficiency motors. However, because the materials are exposed to repeated thermal shock due to ultrafast heating/cooling during L-PBF, it is still challenging to fabricate the dense Nd-Fe-B magnet by using L-PBF. In this study, a high-density (>96%) Nd-Fe-B magnet were successfully fabricated by L-PBF machine. In order to obtain a dense Nd-Fe-B magnet, the substrate pre-heating was performed to reduce the thermal residual stress on the processed sample during L-PBF. Furthermore, the magnetic property of L-PBFed Nd-Fe-B magnet was characterized with microstructure analysis.

**Keywords:** Nd-Fe-B magnet, Additive manufacturing, Substrate-heating, Microstructure, Magnetic property

# Numerical Simulation and Analytical Modeling of Temperature and Morphology of Meltpool in Electron Beam Powder Bed Fusion of Copper Components

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## Abstract

In this research, a numerical study on the prediction of meltpool temperature of Electron Beam Powder Bed Fusion (EB-PBF) of copper has been completed. Two different methods including an analytical model and a numerical simulation tool were performed to estimate the temperature and morphology of the meltpool such as conduction and keyhole mode for this process. The analytical model was developed based on process parameters (beam power and speed) and thermophysical properties of the material. Since the heat transfer of copper is substantially higher than for most metals, the analytical model was developed with heat transfer this factor, and the results were compared with numerical results. The experimental tests were performed to verify both the analytical model and numerical simulations. Results demonstrated that the developed analytical model containing conduction of the material has great accuracy. Statistical analysis demonstrated both beam power and speed have a significant effect on the width, depth, and meltpool temperature for EB-PBF of copper. The proposed model and simulation can be useful to predict the meltpool morphology (conduction to keyhole mode) which drives the bonding quality of the subsequent layer on the overall quality of the printed parts.

**Keywords:** Additive manufacturing, Electron beam powder bed fusion, Meltpool temperature, Simulation, Analytical model

# POSTER Session 2

## Symposium F : Thin Films and Surface Engineering

**P-F0328** **Protective coating of precious metal films on high-melting-temperature metals by chemical vapor deposition**
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**P-F0385** **Environment-Friendly Surface Modification Technology to Strengthen the Steel Surface**
Masataka Ijiri (Tokyo Metropolitan University, Korea)

**P-F0471** **Improvement of Oxidation Resistance in Reduction Sinter-bonding Focusing on Morphology Control of Cuprous Oxide**
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Joonbong Lee (Sejong University, Korea)

| P-F0328 |

# Protective coating of precious metal films on high-melting-temperature metals by chemical vapor deposition

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## Abstract

Chemical vapor deposition (CVD) of precious metals is of great significance for practical applications in electronics, protective coating and catalyst industries. The potential for applications is due to the valuable combination of the intrinsic properties of these metals, including high thermal/chemical stability, high electrical conductivity, and catalytic activity. CVD of precious metals is of interest in preparing oxidation protective coatings on high-melting-temperature metals such as molybdenum (Mo). Iridium (Ir) has a high melting temperature and can be a candidate for CVD coating.

Ir coatings were conducted in a cold-wall CVD reactor equipped with a carbon resistive heater. Mo plates were used as a metal substrate and installed in the reactor. The temperature of the substrate was measured using an infrared thermometer. Argon (99.9999%) was used as a carrier gas and hydrogen (99.999%) as a reducing gas, with their flow rate determined using an electronic mass-flowmeter. An Ir acetylacetonate, Ir(acac)3 precursor, was used as the source material. After the Mo substrate was heated to 1273-1473 K, the evaporated precursor was transported into the chamber with argon and hydrogen gas and the chamber was evacuated to 200 Pa. The phase of Ir films was identified by X-ray diffraction and it was found that the initial phase of the films was Ir-Mo alloy compound such as Mo3Ir and Ir1.02Mo0.98. The cross section of the Ir films was processed by ion milling and a BSE image was obtained. At the presentation, we will report detailed results of Ir coating and its characterization.

**Keywords:** CVD, iridium, protective coating, molybdenum

| P-F0385 |

# Environment-Friendly Surface Modification Technology to Strengthen the Steel Surface

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## Abstract

Rust tends to occur on steel surfaces in relatively clean water, such as river water and tap water, due to oxygen and carbon gas dissolved in the water. Therefore, it is important to prevent water or oxygen from coming into contact with the steel surface in order to prevent the formation of rust. Anti-corrosion measures such as zinc plating, electroless nickel plating, and hard chrome plating are often applied to steel surfaces for this purpose. On the other hand, fine particle peening techniques can also be used to add rust-resistant elements to a steel surface. However, when considering the environmental load of surface modification technologies, waste liquid after plating and the disposal of rare metal particles become problematic. In the study, the effect of mechanochemical multifunction cavitation (MC-MFC) using a sodium hypochlorite solution on the corrosion resistance of low-alloy steel was investigated. The MC-MFC treated surface showed almost no red rust, in contrast to the conventional MFC treated surface. α-FeOOH and β-FeOOH compounds were formed on the steel surface processed by MFC and MC-MFC. In the case of MC-MFC, it was concluded that the amount of β-FeOOH was relatively large because very little formation of red rust occurred. Black and red areas were observed on the unprocessed and MC-MFC processed surfaces after the combined cycle test. From a GD-OES analysis, the MC-MFC treatment was determined to be effective at suppressing rust formation because the amount of Fe compounds was small in the depth direction.

**Keywords:** Multifunction cavitation, Sodium hypochlorite, Cr-Mo steel, Combined cyclic corrosion test, Surface potential

# Improvement of Oxidation Resistance in Reduction Sinter-bonding Focusing on Morphology Control of Cuprous Oxide

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## Abstract

Sinter-bonding using metal particles has been considered to accommodate the operating conditions for wide bandgap semiconductors. In particular, copper particles recently attract attention due to their low cost and their durability against thermal environment. Cu usually oxidizes at low temperatures of 200-250 °C, reducing the sinterability of particles. Therefore, Cu-Cu bonding using Cu particles often requires the inert or reducing atmospheres such as nitrogen or gaseous formic acid to obtain the Cu oxidation resistance, but the bonding in atmospheres presents challenges in terms of cost and safety. In this study, we aimed to realize the Cu-Cu sinter-bonding regardless of bonding atmosphere by controlling surface morphology of Cu particles and the reducing solvent. Anti-oxidation Cu sinter-bonding assisted by low pressure was achieved by using a paste mixed with surface-oxidized Cu particles and polyethylene glycol 400 as a reducing solvent. Cu particles without surface oxidation produced a sparse sintered layer, resulting in the oxidation and fracture of the layer. On the other hand, surface oxidation of Cu particle led to in situ generation of Cu nanoparticles through the reduction by the solvent, which facilitated the densification of sintered layer. The shear strength of Cu joints was retained even after thermal aging at 250 °C in air. It was suggested that the residual organic matter on the surface of sintered Cu played a role in suppressing the oxidation after the bonding process. The high temperature reliable bonding process without atmosphere control could be obtained by considering appropriate particle morphology and solvents.

**Keywords:** Copper, Sintering, Solvent reduction, Anti-oxidation

| P-F0616 |

# Enhanced Accuracy in Hydrogen Sensing by Oxygen Selective Polymer Membrane Support

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## Abstract

The widespread adoption and advancements in hydrogen mobility, particularly fuel cell vehicles (FCVs) and fuel cell forklifts, have led to diverse performance requirements for hydrogen sensors. In response, we have developed a novel hydrogen sensor that combines the electrochemical concentration cell and the functionality of hydrogen-permeable metal membranes, which is the "selective dissolution and diffusion of hydrogen." The sensor consists of a Pd alloy sample electrode deposited on a polymer membrane support, a Pd-H standard electrode, and an electrolyte. The hydrogen sensor can accurately measure gaseous hydrogen concentration and hydrogen in gases containing water vapor or combustible gases. The sensor can also be immersed in a liquid to measure dissolved hydrogen in the liquid directly. However, the output value of the sensor is significantly affected by the oxygen contained in the measurement gas.

In this study, we investigate the effects of the oxygen permeability of the polymer support on the sensor output value. We aim to enhance measurement accuracy by selecting an optimal polymer membrane with oxygen separation capability. Additionally, we explore the influence of polymer membrane thickness on sensor performance.

**Keywords:** Hydrogen Sensor, hydrogen-permeable metal membrane, Dissolved Hydrogen, Oxygen selective polymer membrane

| P-F0640 |

# Refinement of orientation of Sm(Fe,Co)-B thin films by introduction of Sm seed layer

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## Abstract

Sm(Fe-Co)based compounds with the ThMn12-type crystal structure are one of the promising materials to develop high performance permanent magnets due to their excellent intrinsic magnetic properties. Recently, we reported that the addition of B to Sm(Fe-Co) thin films led to the formation a B-rich grain boundary (GB) phase and significantly improved the coercivity μ0Hc. Moreover, μ0Hc was further increased by Si diffusion from the cap layer into GB phase. However, it was predicted that not only GB diffusion but also suppression of soft magnetic phase existing between V under layer and Sm(Fe,Co)-B layer play important role to achieve a high μ0Hc. In this study, in order to reduce the amount of soft magnetic α-Fe(Co) phase, the crystal structure and magnetic properties of Sm(Fe,Co)-B thin films with Sm seed layer have been investigated in detail. The samples were prepared by using an ultra-high vacuum magnetron sputtering system. First of all, V under layer was deposited on MgO(100) substrate. Subsequently, a Sm seed layer and Sm(Fe,Co)-B were deposited. Finally, V cap layer was deposited to prevent from oxidation of thin films. The crystal structure of thin films was determined by XRD, the magnetization curves were measured by SQUID. From the XRD patterns, the (002) and (004) peaks from the ThMn12-type crystal structure of main phase were obtained for all the samples. Intensity of the peaks from main phase were increased but intensity of the peak from α-Fe(Co) phase was reduced by introducing a Sm seed layer.

**Keywords :** α-Fe phase, coercivity, RFe12 compounds, ThMn12-type structure

# Comparison of Fe-Ni Alloy Films Fabricated by DC, Two-Step and Pulse Electrodeposition

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## Abstract

Electrodeposition of Fe-Ni invar alloy has advantages in fabrication of thin film with low cost compared to traditional process like rolling. However, the properties of the electrodeposited films along the thickness direction are different due to anomalous behavior of Fe-Ni codeposition and they are affected by various factors such as bath composition, current density, and current waveform. In this research, Fe-Ni films were fabricated on mirrored Titanium substrate with direct current (DC), two-step and pulse current (PC) electrodeposition techniques. The Fe-Ni films of invar composition (36-40 wt% Ni) fabricated by DC electrodeposition had rough surface and mixed structure of FCC and BCC. To enhance surface morphology of deposits, the two-step and PC electrodeposition were conducted at various conditions of first step and the average current density and frequency of PC, respectively. In addition, to investigate difference in front and back of the deposits, the composition and microstructure of both surfaces were analyzed by EDS and XRD.

**Keywords:** Fe-Ni invar alloy, Two-step electrodeposition, pulse electrodeposition

| P-F0820 |

# Preliminarily exploring the electrical insulation performance of APPJ $SiO_2$ coating on 304 stainless steel pipes

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## Abstract

The atmospheric pressure plasma jet technique is used to prepare SiO2 insulation coatings onto the outer surface of 304 stainless steel pipes (304-SSPs). The diameter and surface roughness of 304-SSPs increase from 18 to 32 mm and 0.1 to 1.0 μm. The results show that the atmospheric pressure plasma jet scanning methods have little influence on the chemical composition, chemical bond structure, crystal structure, and surface morphology of SiO2 coatings, which display Si/O=1/(1.95±0.02), dominant Si-O bond, amorphous structure, and dense layer structure. However, the atmospheric pressure plasma jet scanning methods have obvious influence on the uniformity and electrical insulation resistance (REI) of SiO2 coatings. Only when the atmospheric pressure plasma jet is parallel to the normal direction of 304-SSPs outer surface, the balance between atmospheric pressure plasma jet impingement, gravity, and coating surface tension could reach the optimal condition, which improves the uniformity and REI of SiO2 coatings. With the optimal scanning method, REI of SiO2 coatings decrease with the increase of surface roughness of 304-SSPs, which are caused by the decrease of effective thickness of SiO2 coatings. Most importantly, with the other parameters as constant, REI of SiO2 coatings reaches to ~101 MΩ and displays the better uniformity when the diameter of 304-SSPs is about 5 times the diameter of atmospheric pressure plasma jet tube.

**Keywords:** Electrical insulation resistance; SiO2 coating; Atmospheric pressure plasma jet; Outer wall; Stainless steel pipe

| P-F0821 |

# Investigate the heat conduction between film and substrate during sputtering process by multi-layer structure NiCr/NiSi film thermocouples

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## Abstract

The three layers of structure NiCr/NiSi film thermocouples were deposited onto the glass substrate by the direct current pulsed magnetron sputtering technique. The hot junctions of three film thermocouples were overlapped. Between the hot junctions, SiO2 insulation films were deposited. Then, the heat conduction between TiO2 film and substrate was investigated. The results showed that at the initial stage of TiO2 film growth, the electromotive force (EMF) of top film thermocouple was higher than that of middle film thermocouple. The electromotive force difference between top and middle film thermocouples increased with time. Meanwhile, the electromotive force of bottom film thermocouple was also higher than that of middle film thermocouple. The electromotive force difference between bottom and middle film thermocouples increased with time. Until the critical time, the middle film thermocouple received the heat conduction from TiO2 film and substrate. At the critical time, the electromotive force difference between top and middle film thermocouples, as well as between bottom and middle film thermocouples, reached the maximum, which meant the heat conduction equilibrium state between top, middle, and bottom film thermocouples. Then, because of the heat conduction from hot junction to pads of TFTCs, the electromotive force difference between top and middle film thermocouples, as well as between bottom and middle film thermocouples, both decreased with time.

**Keywords:** Film thermocouple; Heat conduction; Film growth surface; Sputtering

| P-F0979 |

# Microstructure characterization of Zn-15Al-6Mg-0.2Si alloy galvanized coating

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## Abstract

We investigate the microstructure of Zn-15Al-6Mg-0.2Si coating layer of galvanized steel sheet utilizing thermodynamic calculations, X-ray diffraction, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Vickers hardness tests. It is observed that the FeAl intermetallic layers are present between the coating layer and Fe matrix. The FeAl layer is identified as Al12Fe7 phase with a preferred growth direction for the Fe matrix. Thermodynamic calculation indicates that the primary Mg2Si, MgZn2 and f.c.c. Al phases form in the coating layer prior to the formation of h.c.p. Zn matrix. Metallographic analysis shows that the areal fractions of Mg2Si, MgZn2, Al, and Zn/Mg2Zn/Al ternary eutectic phases are 8.4%, 13.0%, 53.1%, and 25.6%, respectively. The crystal structure, internal precipitate, and orientation relationship of the phases were further examined by TEM. There are crystallographic orientation relationships between primary Mg2Si, MgZn2, and Al phases. This indicates the heterogeneous nucleation of primary phases, which is related to serial formation of primary phases upon solidification. The primary f.c.c. Al phase is divided into two parts with different Zn concentrations, which results from Zn enrichment during solidification. The size and fraction of Zn precipitates are higher in the Al phase with higher Zn concentrations. The η-MgZn2 precipitates and its metastable η' precipitates are additionally observed in the primary Al phase. Meanwhile, the primary MgZn2 phase contains nanoscale Mg2Zn11 phase. The relationship between constituting phases and hardness of coating layer is discussed.

**Keywords:** Galvanized steel, Galvanzing, Zn-Al-Mg-Si coating, Transmission electron microscopy, Microstructure characterization

| P-F1056 |

# Regeneration of single-walled carbon nanotube membranes for optical applications in the extreme ultraviolet range

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## Abstract

We propose a facile, cost-efficient, environmentally friendly, and scalable process for the regeneration of single-walled carbon nanotube membranes serving as extreme ultraviolet (EUV) protective pellicles. The method comprises of high-temperature treatment of the membrane by Joule (resistive) heating at 1400 °C and pressure below 3×10-1 Pa. Using model Sn aerosol nanoparticles, the primary contaminant from extreme ultraviolet light sources, we demonstrate the proposed method to clean the membrane with the power consumption as low as 20 W/cm2. We show the proposed method to cause no harm to carbon nanotube structure, opening a route towards multiple membrane regeneration. We confirm the applicability of the approach using in situ deposition from the EUV light source and subsequent Sn aerosol contaminant removal, which restores the EUV-UV-vis-NIR transmittance of the film and therefore the light source performance. The proposed method supports pulse-cycling opening an avenue for enhanced protection of the lithography mask and stable performance of the EUV light source. Additionally, the approach is suitable to other composite contaminants in a form of nanoparticles based on such species as Pb, In, Sb, etc.

This work was supported by a grant of the Russian Federation MK-3000.2022.1.3 and the Russian Science Foundation (project No. 21-72-20050).

**Keywords:** Single-walled carbon nanotubes, pellicle, thin films, EUV lithography

| P-F1165 |

# Surface and Interface Engineering of Oxide Hard Coating for High-performance Cutting Tool

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## Abstract

Advanced cutting tools for difficult-to-cut work piece materials (i.e. titanium alloy) need long life time during cutting process to require more accurate process and lower production costs. Extra hard coating layers, consisted of nitride, oxide and carbide, can be adopted to improve their cutting performances and wear resistance during cutting process. Metal nitride hard coatings, such as TiN and CrN, have uncontrollable oxidation layer and internal thermal stress issues which can be caused poor life time. In this work, in order to improve coating properties nano-crystalline oxide hard coating on cutting tool which consisted metal nitride coated on WC. Indeed, such a nano-crystalline oxide layers improve mechanical properties (hardness, elastic modulus, internal stress and oxidation resistance), enhancing tool life time. Furthermore, an interfacial layer is adopted between nitride and oxide hard coating to improve their surface profile and adhesion.

**Keywords:** Hard coating, Oxide thin film, Surface and interface engineering, Cutting tool, Difficult-to-cut

# POSTER Session 2

## Symposium G : Materials for Energy Storage and Generation

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Seoyeon Park (Korea University, Korea)

# Competition between charge collection and recombination dynamics in polymer/polymer solar cells

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## Abstract

It is well known that there is a trade-off relationship between an increase in short-circuit current density (JSC) and a decrease in fill factor (FF) as the film thickness increases in polymer/polymer solar cells. Here, we focused on polymer/polymer solar cells based on three donor polymers with different side chains (J51, J61, and J71) and an acceptor polymer (N2200) to discuss how charge collection and recombination impact on FF in thick films. For the J51/N2200 and J61/N2200 devices, FF was drastically degraded down to 0.4 in thick films, while that of the J71/N2200 was only slightly decreased and maintained as high as 0.6. To discuss the origin of these trends, we analyzed the recombination dynamics measured by transient optoelectronic techniques. From the experimental data obtained, we estimated the recombination reduction factor (ζ), which is a measure of suppressed bimolecular recombination. For all the devices, ζ was evaluated to be about of the order of 10–2, suggesting well-suppressed bimolecular recombination. On the basis of these recombination dynamics, we reconstructed the current density–voltage curves to examine how they impact on FF. The reconstruction result shows that only J71/N2200 device was well-reconstructed, indicating that FF is dominated by bimolecular recombination. In contrast, the other devices were not well-reconstructed because the carrier density was underestimated for these two devices. Interestingly, the reconstructed curves are well-reproduced by considering additional charge carriers, implying that there is an additional recombination driven by isolated charge carriers. We will further discuss the effect of competition between charge collection and recombination on FF.

**Keywords:** polymer/polymer solar cells, charge collection/recombination, charge transport properties, fill factor

| P-G0311 |

# Effect of lattice defects on hydrogenation behavior in HfNbTiZr medium entropy alloy

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## Abstract

Hydrogen storage alloys, a class of alloys capable of absorbing and releasing hydrogen through reversible reactions, have received considerable attentions in recent years due to their potential application in energy storage. Severe plastic deformation (SPD) processes, such as high-pressure torsion (HPT), have been reported to accelerate the hydrogenation kinetics in hydrogen storage alloys by introducing lattice defects (vacancies, dislocations, and grain boundaries). This suggests that the microstructures of materials affect the hydrogenation behavior although the exact contributions of each defect and the underlying mechanisms remain unclear. This study aims to elucidate the contributions of each lattice defect on the hydrogen storage properties of a HfNbTiZr medium entropy alloy (MEA) with a body-centered cubic structure by systematically investigating the relationship between the hydrogenation behavior and microstructures in SPD-processed and recrystallized specimens with different grain sizes. Ingots of the MEA were subjected to HPT with five rotations at room temperature. The as-HPT materials were then annealed at different temperatures for different periods to obtain fully recrystallized microstructures with different average grain sizes. The pressure-composition isotherms of the as-HPT and recrystallized samples were evaluated electrochemically by cathodic polarization in a 6 M KOH aqueous solution using a constant current. It was found that fully recrystallized specimens exhibited a limited hydrogen capacity, while the hydrogen capacity greatly increased after HPT. The results suggest that lattice defects introduced by HPT significantly affect the hydrogenation behavior of the MEA. In the presentation, the roles of each lattice defect to the hydrogenation properties will be also discussed.

**Keywords:** Hydrogen storage alloys, High/Medium entropy alloys, Severe plastic deformation, Lattice defects, Electrochemical characterization.

| P-G0314 |

# Helium and hydrogen effect of cavity formation and irradiation hardening on CrFeNiMn high entropy alloy and 316 stainless steel

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## Abstract

In recent years, high-entropy alloys (HEAs) have attracted attention due to their excellent mechanical property and high irradiation resistance. People have investigated the irradiation effect of HEAs using heavy ion irradiation, but the helium and hydrogen effect on HEAs has not been studied enough so far. In this study, we conducted single beam (Fe), dual beam (Fe+He), and triple beam (Fe+He+H) irradiation experiment on Cr0.8FeMnNi and 316L, and then use nano-indentation and TEM method to characterize. According to TEM results, there were cavities formed in Cr0.8FeMnNi after irradiation, but the size, shape and distributed depth are different with irradiation beam. The cavities of Fe irradiated samples are larger and with lower density compared with triple beam irradiated samples at 1 μm, where He and H distributed. Also, the cavities in triple-irradiated-samples formed at deeper depth and showed different distributed patterns: parallel to radiation direction, perpendicular to radiation direction and random distribution. This might result from the synergistic effect of helium and hydrogen. He and H can attract and stabilize vacancies, so the migration of vacancies is depressed and small cavities formed because of the presence of He and H. From nano-indentation test results, we found the hardness increment of Cr0.8FeMnNi under different irradiation condition is smaller than that of 316L. But in triple beam irradiated samples, irradiation softening occurs, which might because the element segregation and the formation of Cr-Mn-O oxide on the surface.

**Keywords:** High entropy alloy; Helium and hydrogen effect; Cavity; Irradiation softening.

| P-G0635 |

# Fabrication and Characteristic of Oxide Dispersion Strengthened Ferritic Steels Containing Gadolinium Oxide for Neutron Absorbing Structural Components

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## Abstract

Gadolinium (Gd) is well known that a neutron absorbing element exhibits approximately 67 times superior in a neutron absorption capacity compared to boron. In recent studies, Gd is being added as an alloying element to stainless steels to have excellent neutron absorbing capacity for a spent fuel storage. While this showed high neutron absorption capacity, Gd forms brittle intermetallic phase such as M3Gd due to very low solubility in Fe-Cr matrix, which eventually results significant decrease of hot workability and corrosion resistance. Additionally, it had a trade-off relationship in the mechanical properties, as the amount of Gd increased, yield strength and elongation significantly decreased. In this study, gadolinium oxide (Gd2O3) distributed ferritic stainless steels with excellent mechanical properties, corrosion resistance as neutron absorbing structural components were instantly fabricated and their characteristics were carried out. Oxide dispersion strengthening is one of the most promising ways to improve the mechanical property at elevated temperatures in many alloy systems. Since Gd2O3 particles were uniformly distributed with a high number density, it could be expected that a formation of unfavourable intermetallic phase was sufficiently suppressed. Mechanical Alloying, hot isotactic pressing, and hot rolling processes were employed to fabricated sheet and plate specimens. And then their microstructures and tensile properties at elevated temperatures were also investigated. Experimental results suggest a promising applicability of ODS ferritic steels for the neutron absorbing structural materials with higher mechanical properties and corrosion resistance.

**Keywords:** Gadolinium Oxide, Neutron Absorbing Material, Powder metallurgy, ODS steel, Tensile Property

| P-G0850 |

# Cu-promoted non-noble catalysts for the efficient hydrolysis of ammonia borane

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## Abstract

Highly efficient and cheap catalysts for room-temperature hydrolysis of ammonia borane (AB) is of great signifificance for their real application in hydrogen (H2)-based fuel cells. Here, we report a faciel and efficient synthesis of Cu based-non-noble metal nanoclusters and demonstrate their high catalytic performance toward the hydrolysis of AB, which is achieved through direct carbothermal shock pyrolysis of metal precursors in just ~100 ms. We find that the optimum Cu0.04@ZIF67 achieves a superior catalytic activity with a turnover frequency of 400 molH2 molCu −1 min−1 in 1 M NaOH, better than most of previously reported non-noble nanocatalysts. It also exhibits a very low activation energy (Ea) of 35.4 kJ mol−1. The studies show that the high activity is attributed to the synergistically structural and compositional advantages of Cu and Co in ZIF-67. The low cost, superior catalytic performance and efficient synthesis methods provides an opportunity for their practical application in chemical hydrogen storage.

**Keywords:** Hydrogen production, Ammonia borane, Hydrolysis, carbothermal shock Catalytic kinetics

# Betavoltaic-powered electrochemical cells based on $TiO_2$ Nanotubes modified with $ZrO_2$ and SWCNTs

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## Abstract

Focusing on the demand of nuclear cells with long-life and high-reliability in the aerospace field, this study explores the optimization of Betavoltaic-powered electrochemical cells (BPECs) to efficiently convert the decay energy of radioisotope to the electrical energy. The BPEC was fabricated using titanium dioxide (TiO2) nanotube arrays (TNAs) that were modified with zirconium oxide (ZrO2) nanoparticles and single-walled carbon nanotubes (SWCNTs). The calculated efficiency can reach 15.03% when using effective energy deposition that was obtained by the Geant4 simulation. Experimentally, the conversion efficiency of the optimized BPEC can reach 12.76%, which is nearly three times higher than that using simple TNAs. The open-circuit voltage (Voc) is 291.53 mV, and the maximum power (Pmax) can reach 131.44 nW/cm2 under the radiation of 63Ni radioisotope source (10 mCi/cm2). The enhanced mechanisms of BPEC can be attributed to the formation of TiO2/ZrO2 heterojunction with Type-I band alignment, which is helpful for the interface carrier separation and the suppression of carrier recombination. In addition, the organic electrolyte ($I^-/I3^-$) injected into the TiO2 nanotube channel, and the formation of a three-dimensional solid-liquid heterojunction effectively separates the radiation-generated electron-hole pairs, allowing electrons to be transferred from the TiO2 nanotube wall to the Ti substrate and holes to be transferred to the electrolyte via the TiO2 and SWCNTs surfaces to participate in the redox reaction. Electrons and holes have distinct transport routes, which helps to prevent carrier recombination. This study provides a new strategy for improving the conversion efficiency of radio-voltaic cells.

**Key words:** Betavoltaic-powered electrochemical cell, TiO2 nanotubes, Radioisotope, nuclear battery.

| P-G0944 |

# Development of hot rolling on La-Fe-Co-Si magneto-caloric composites

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## Abstract

Magnetocaloric materials (MCMs) have the advantages of high energy efficiency and environmentally friendly cooling technology compared to conventional vapor-cycle refrigeration. However, there is a certain limit to commercializing magnetic refrigeration because existing systems are still getting low cooling efficiency with imperfect heat exchanger structures, such as powder packing structures. To improve the performance of the magnetic refrigeration, a magneto-caloric regenerator needs to have as much heat exchange area as possible with minimizing pressure drop. In this study, we develop the hot rolling process as part of the MCM componentization technology. La-Fe-Co-Si alloy was utilized for the hot rolling process, and we also designed La-Fe(11.2-x)-Co(0.7+x)-Si1.1 (x=0 – 0.5) alloy by controlling Co (0.7 – 1.1 atomic ratio) content to diversify the Curie temperature. We achieved a compression ratio of up to 87% below the 1 mm thickness sheet by hot rolling, and the influence of the compression ratio on the MCM properties was analyzed. In addition, the microstructural evolution of the La-Fe-Co-Si alloy was characterized from casting to hot rolling to MCM heat treatment state with the magneto-caloric effect. Finally, we develop the bulk deformation hot rolling process for magnetocaloric materials to fabricate the La-based MCM sheet and consequently verify the possibility of bulk MCM forming (e.g. sheet and plate) for the componentization of magnetic regenerator.

**Keywords:** La-Fe-Co-Si alloys, Hot rolling process, Magnetocaloric effect, NaZn13-type phase

| P-G0950 |

# Forming Technology of Anisotropic Gadolinium wire and Componentization of Active Magnetic Regenerator

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## Abstract

Recently, there has been increasing attention on environmentally friendly research due to the emergence of carbon neutrality policies aimed at reducing greenhouse gas emissions. In this regard, magnetocaloric materials (MCM) are potential candidates for eco-friendly systems. In order to raise the efficiency of the magnetic refrigeration system to the level of conventional gas refrigerators so that it can be commercialized in reality, forming technology of MCM and subsequent componentization should be required. In this study, we developed the multi-pass drawing process for monolithic gadolinium (Gd) to fabricate the Gd wire assembly. With the multi-pass drawing process, we figured out the magneto-anisotropic properties of Gd wire depending on the forming direction. The microstructural evolution of c-axis orientation was developed perpendicular to the drawing direction, and identified via EBSD and SEM analysis. In addition, we designed the wire assembly and micro-channel for the magnetic regenerator and quantitatively investigated the pressure drop and heat transfer rates depending on the geometry parameters such as the hole size of the micro-channel and diameter of the wire through ANSYS Fluent simulation.

Finally, we have confirmed for the first time the magneto-anisotropic properties resulting from the Gd drawing process and observed the potential of bulk forming technology for MCM.

**Keywords:** MCM(Magnetocaloric Materials), MCE(Magnetocaloric Effect), Drawing, Forming technology, Magneto-anisotropic

# $Fe_{1-x}S$ modulated by sulfur sources for high-performance anodes in Li-ion batteries

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## Abstract

The commercial lithium-ion batteries (LIBs) based on anode materials of graphite can not meet the continuously rising for high power or energy densities from portable electric devices and newly emerging large-scale applications. It is urgent to develop new anode materials with higher specific capacity. Electrodes based on conversion reaction supply generally exhibit a high specific capacity larger than 500 mAh/g with a mild volume change after lithiation. In this work, Fe1-xS was synthesized by the direct calcination of Fe2O3 and different sulfur sources (thioacetamide and thiourea) for anode material of LIBs. Fe1-xS synthesized using thioacetamide has a reversible capacity of 524 mAh/g at 100 mA/g, while the specific capacity of Fe1-xS synthesized using thiourea is only 402 mAh/g. The mechanism for the difference is also explored to highlight the importance of surface modification on these conversion-type electrodes.

**Keywords:** Li-ion batteries, iron sulfide, Conversion reaction, electrochemistry.

| P-G1045 |

# Elevated temperature design of Type 316L stainless steel components and piping in a thermal energy storage system

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## Abstract

In elevated temperature design of a large-scale 700°C thermal energy storage test facility (called TESET) under construction at KAERI(Korea Atomic Energy Research Institute), Type 316L stainless steel has been applied as heat resistant structural material. 316L SS has been selected because it is economical and the readily available. The TESET facility uses sodium as coolant with operating temperature of 700°C at atmospheric pressure for thermal energy storage from renewable energy sources such as concentrated solar thermal energy. In the design and construction of 700°C thermal energy storage facility, French nuclear design rules of RCC-MRx were used with supplementary works on insufficient material properties around 700°C. In ASME codes such as ASME Section VIII or Section III Division 5, elevated temperature material properties are not available for 316L SS, which is why it is not possible to apply ASME codes while RCC-MRx provides high temperature material properties in the creep range. However, as elevated temperature material properties such as creep rupture strengths are not fully provided up to the temperature of 700°C, a series of material tests on tension, fatigue and fracture toughness over the temperatures up to 700°C were conducted for the determination of the insufficient material properties for 316L SS in RCC-MRx. The design evaluation results based on a number material tests and supplementation works for lack of material properties showed that an application of 316L SS to 700°C thermal energy storage system was shown to be possible over a limited time duration.

**Keywords:** High-temperature design, Type 316L stainless steel, Thermal energy storage, Pressure boundary components and piping, Creep-fatigue.

| P-G1128 |

# Multifunctional Composite Platforms Based on Binder-free Graphene Oxide Dough

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## Abstract

Graphene-based composites, which combine the exceptional properties of graphene with other functional materials, have garnered significant attention for a wide range of applications. The construction of such composites requires easy-incorporation and homogeneous distribution of functional materials without compromising their inherent properties. Here, we present a facile strategy for fabricating dense and versatile graphene composites by directly integrating GO and nanopowders without any binders and extra process. The GO doughs (GODs), derived from highly concentrated GO dispersion, have adhesiveness and thus can be readily, uniformly, and physically mixed with solid nanopowders to enhance functionalities. The composite GODs are formable, allowing for the design of structures suitable for various applications. The resulting reduced GOD (RGOD)-based composite films contributed to excellent performance in supercapacitors and electromagnetic interference (EMI) shielding. The RGOD film consisting of RuO2 nanoparticles and CNTs (RuO2@CNT@RGOD) exhibited outstanding electrochemical performance with a high volumetric capacitance of 285 F/cm3 and an excellent cyclic stability of 93 % at 10 A/g after 10,000 cycles. Moreover, the integrated RGOD architectures with CNTs and Fe2O3 nanoparticles and the unique layered sandwich structures of RGOD and Fe2O3 improved EMI shielding effectiveness, leading to the outstanding total EMI SE (SET) up to 81.3 dB. This study offers an innovative approach to manufacturing graphene-based composite materials with exceptional processability for diverse application of next-generation electronics.

**Keywords:** Graphene, Composite, Binder-free, supercapacitor, EMI shielding

# POSTER Session 2

## Symposium H : Electronic and Magnetic Materials

**P-H0103** **Prediction of Supercooled Liquid Region of soft magnetic bulk metallic glasses by Deep Learning**
Chunghee Nam (Hannam University, Korea)

**P-H0284** **Static and High-frequency Magnetic Properties of Toroidal Cores Composed of Electrolytic Iron Particles with Different Shapes**
Yudai Kodama (Tohoku University, Japan)

**P-H0586** **Copper/graphite metal matrix composite for heat management application**
JONGTAE KIM (DGIST, Korea)

**P-H0620** **Quasi first-order magnetic transition of Mn0.9Fe0.1Sb0.9Sn0.1 probed using Mössbauer spectroscopy**
Masahira Onoue (Kagoshima University, Japan)

**P-H0641** **Effect of additive elements on the crystal structure and magnetic properties for L10 Mn-Ga thin films**
Yuto Miura (Tohoku Gakuin University, Japan)

**P-H0876** **Effect of High Efficiency Heat Treatment System on Magnetic Properties of Co27 Alloy**
Yan Dongchao (Advanced Technology & Materials Co.,Ltd., China)

**P-H0897** **A study on the magnetic properties and magnetocaloric effect of Tm1-xErxCuAl (x=0, 0.2, 0.4, 0.5, 0.6, 0.8, 1) polycrystalline compounds**
Sun Hao (University of Science And Technology Of China, China)

| P-H0103 |

# Prediction of Supercooled Liquid Region of Soft Magnetic Metallic Glasses by Deep Learning

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## Abstract

In this study, the supercooled liquid region (ΔTx) of Fe-based metallic glasses was predicted using a convolutional neural network (CNN), which is one of the popular deep-learning models. ΔTx is defined as Tx-Tg, where Tx is the onset crystallization temperature and Tg is the glass temperature. ΔTx can be considered a characteristic indicator of thermally stable bulk metallic glass. CNN-guided supervised learning was performed using only the compositional features without structural information and physics-informed features. The chemical formula in the material dataset was used to generate 140 features with the python libraries 'Pymatgen' and 'Matminer'. The regression performance to predict ΔTx was evaluated using the determination coefficient (R2 score) and root-mean-squared errors (RMSE). For the CNN network, various input shapes of 140 compositional features were employed as the input vectors, including 10 × 14, 14 × 10, 7 × 20, and 20 × 7. Among them, the 14 × 10 compositional feature vectors exhibited the best prediction performance for ΔTx with an R2 score of 0.924 and RMSE of 7.7 K . As a case study, the trained CNN model was applied to predict ΔTx of recently developed Fe-based metallic glasses, corresponding to unseen datasets. The predictions of the unseen datasets were found to be in excellent agreement with the reported experimental results for ΔTx, indicating that the composition-based CNN model opens a new path to search for promising Fe-based metallic glasses with high glass-forming ability.

**Keywords:** deep learning, Fe-based metallic glasses, supercooled liquid region

| P-H0284 |

# Static and High-frequency Magnetic Properties of Toroidal Cores Composed of Electrolytic Iron Particles with Different Shapes

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## Abstract

To achieve next generated power electronics devices, passive devices such as transformer, inductor and so on are required to be highly efficient and compact. In particular, iron-based dust core has been getting attention as one of the soft magnetic materials for passive devices because of their high saturation magnetization and low iron loss. Herein, we selected electrolytic iron particles with different shapes (needle, flat, and spherical) as a newly soft magnetic material for toroidal cores, investigated static and high frequency magnetic properties of toroidal cores composed of these particles in detail, and discussed the effect of the particle shape on these properties.

The toroidal core composed of spherical particles had the highest saturation magnetic flux density and permeability, while the toroidal core composed of needle particles had the highest coercivity in all cores. The reason for these behaviors is difference in volume for the cores.

For every core, the core loss almost kept constant in the low frequency range, while increased due to eddy current loss in the high frequency range. For the toroidal core composed of flat particles, the frequency at which the core loss increased became highest in all cores, and then its core loss became lowest in the high frequency range. The reason for this is that small cross-sectional areas with flat particles reduced eddy current flow.

Therefore, these results suggest that both static and high-frequency magnetic properties of dust cores can be designed by controlling particles shape.

**Keywords:** Magnetic cores, Magnetic losses, Soft magnetic materials, Electrolytic iron powder.

# Copper/graphite metal matrix composite for heat management application

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## Abstract

Copper/graphite (Cu/Gr) metal matrix composites have attracted attention for thermal management applications due to their high thermal conductivity (TC) and low coefficient of thermal expansion (CTE) values. This study investigates the thermal and mechanical properties of reinforced metal matrix composites (Cu/Gr) and their dependence on the content (5-60v%) and crystal orientation of the reinforced material (Gr). Using a spark plasma sintering (SPS) technique, the composite material was fabricated by sintering for 10 minutes after raising the temperature to 650-850°C at a heating rate of 120°C/min under a pressure of 50-80 MPa. The crystal orientation was analyzed using an X-ray diffractometer (XRD) and field emission scanning electron microscopy (FE-SEM). TC and CTE of the sample were measured using a laser flash analyzer (LFA) and a thermomechanical analyzer (TMA), respectively. The XRD and FE-SEM analysis confirmed that the graphite crystalline orientation in the composite material was perpendicular to the pressing direction of the SPS sintering. Furthermore, analysis of thermal conductivity in the composite samples revealed that the sample with 5v% of graphite, pressed in the direction perpendicular to the basal plane, exhibited the highest thermal conductivity (479.21W/m·K) which is higher than that of bulk Cu (398W/m·K). However, the thermal conductivity decreased when the Gr filler content was further increased. The CTE of the composites was in a range between 11.24 and 13.63 ppm/K which is lower than that of bulk Cu (16.7 ppm/K). There existed no clear dependence of the CTE on the crystal orientation of the Gr fillers.

This work was supported by the DGIST R&D Program of the Ministry of Science and ICT of Korea (23-ET-07).

**Keywords:** Copper/Graphite, Metal matrix composite, Thermal conductivity, Crystal orientation

| P-H0620 |

# Quasi first-order magnetic transition of Mn0.9Fe0.1Sb0.9Sn0.1 probed using Mössbauer spectroscopy

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## Abstract

Mn2Sb0.9Sn0.1 with a tetragonal Cu2Sb-type structure shows the first-order magnetic transition (FOMT) between ferrimagnetic (FRI) and antiferromagnetic (AFM) phases at about 170 K [1]. In Cu2Sb unit cell, Mn occupies 2a- and 2c-sites, denoted as Mn(I) and Mn(II), respectively. In Mn1.9Fe0.1Sb0.9Sn0.1, in which Mn is substituted with a small amount of Fe, the FOMT between FRI and AFM disappears, and a quasi-first order magnetic transition (Q-FOMT) appears at about 320 K instead [2]. Magnetization and XRD measurements have shown that the Q-FOMT in Mn1.9Fe0.1Sb0.9Sn0.1 is associated with spin reorientation (SR) [3,4]. In this study, 57Fe Mössbauer spectroscopy was performed on Mn1.9Fe0.1Sb0.9Sn0.1 near the Q-FOMT temperature, and the relationship between SR and Q-FOMT was investigated from a microscopic point of view.

Mössbauer spectroscopy revealed that Fe atoms occupy 63% of the 2a-site and 37% of the 2c-site in the Cu2Sb-type structure. The hyperfine field was evaluated as 6.8(2) T for the 2a-site and 4.0(2) T for the 2c-site. The quadrupole splitting (QS) was evaluated as 0.12(4) mm/s for the 2a-site and -0.76(7) mm/s for the 2c-site at room temperature. When the temperature was increased to 313 K, the signs of QS at both sites flipped to -0.11(2) mm/s at the 2a-site and 0.3(2) mm/s at the 2c-site. Sign changes in QS are associated with SR [5]. Therefore, our microscopic results suggest that the Q-FOMT observed in Mn1.9Fe0.1Sb0.9Sn0.1 is related to SR.

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**Keywords:** quasi-first order magnetic transition, spin reorientation, Mössbauer spectroscopy.

| P-H0641 |

# Effect of additive elements on the crystal structure and magnetic properties for L10 Mn-Ga thin films

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## Abstract

The countries of origin of rare earth magnet materials are unevenly distributed, and they are expensive and unstable. Therefore, development of rare-earth-free permanent magnets is strongly needed. Mn-Ga alloy films with L10 structure have attracted much attention for application to rare-earth-free permanent magnets and STT-MRAM. In this study, in order to see the effect of additive elements (N, Fe and Cu) on the crystal structure and magnetic properties of L10 Mn-Ga thin films have been investigated. The samples were prepared on MgO (100) single crystal substrates using an ultra-high vacuum magnetron sputtering system. Mn-Ga thin films with additive elements were deposited at 500 °C. The thickness of film was fixed at 20 nm. After deposition, the substrate was cooled down to room temperature, and all films were capped with 10 nm Cr layer to prevent oxidization. The crystal structure was determined by XRD. The magnetic properties were measured by using a SQUID. From the X-ray diffraction patterns, both the (001) and (002) peaks from the L10 structure of Mn-Ga alloy were clearly observed for all the samples. The coercivity was slightly increased by the addition of small amount of Fe (~ 5.0 vol. %). The intensity of the peak arise from the L10 structure was increased for Mn-Ga-Cu alloy thin films and also the saturation magnetization was significantly increased from 529 (w/o Cu) to 637 emu/cm3. However, no remarkable improvement was observed for the case of N addition.

**Keywords:** Mn-Ga alloy, L10 structure, saturation magnetization, thin film

| P-H0876 |

# 高效热处理制度对Co27合金磁性能的影响

# Effect of High Efficiency Heat Treatment System on Magnetic Properties of Co27 Alloy

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**摘要：**

Co27合金是具有高饱和磁感应强度、高居里温度的软磁材料，被广泛应用于电子设备等领域。通常使用Co27合金，需要经过至少8h的磁退火处理。本文旨研究在生产过程中对Co27合金进行短时热处理，最终产品可不经过磁退火直接使用。研究表明：最佳的短时热处理制度为750℃保温1.5min，此时Co27的磁性能达到最优。磁性能B2400达到国标GB/T 14986.3要求的92%，其余指标均满足国标要求。该磁性能指标完全满足目前声学领域的使用要求，显著提高了生产效率，降低了成本。最佳短时热处理制度下Co27合金的抗拉强度为1040MPa，屈服强度为995MPa，延伸率为6%，硬度值为187（HV1）。

**关键词：**热处理；Co27合金；磁性能；力学性能

**Abstract:**

Co27 alloy was a kind of soft magnetic material with high saturation magnetic induction intensity and high Curly temperature. Co27 alloy was widely used in electronic equipment and other fields. Co27 alloy needed to be magnetically annealed for at least 8 hours. The purpose of the paper was to study the short-term heat treatment of Co27 alloy in the production process. the final product can be used directly without magnetic annealing. Research showed that the best short-term heat treatment system was 750°C for 1.5min, the magnetic performance of Co27 was optimal. The magnetic performance B2400 reached 92% of the requirements of the national standard GB/T 14986.3. The remaining indicators meet the requirements of the national standard. The magnetic performance index fully met the current requirements in the field of acoustics, which significantly improved production efficiency and reduced costs. Under the optimal short-term heat treatment system, the tensile strength of Co27 alloy was 1040MPa, the yield strength was 995MPa, the elongation rate was 6%, and the hardness value was 187 (HV1).

**Key words :** Heat treatment; Co27 alloy; Magnetic properties; Mechanical properties

| P-H0897 |

# A study on the magnetic properties and magnetocaloric effect of $Tm_{1-x}Er_xCuAl$ (x=0, 0.2, 0.4, 0.5, 0.6, 0.8, 1) polycrystalline compounds

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## Abstract

In the past, the influence of the structural orientation and shape factor on magnetic results is often overlooked in the investigation of magnetic and magnetocaloric effects (MCEs) of alloys prepared by arc-melting using the magnetic measurement equipment such as MPMS, VSM, and PPMS, which will result in the non-comparability of the experimental data measured in different states. To address the issue, the direction of the structural orientation and shape factor of Tm1-xErxCuAl (x=0, 0.2, 0.4, 0.5, 0.6, 0.8, 1) polycrystalline compounds prepared by arc-melting are strictly controlled in the experiment by precise machining to be almost identical for each sample. By comparing the magnetic measured results, it is found that the -ΔS_M^max and RC values of Tm1-xErxCuAl increase with increasing x, except for the x=0.5 component. The -ΔS_M^max and RC values are the x=0.5 component exceeds that of the x=0.6 component, which is related to the modulating effect of rare magnetic moment in the c-axis direction. Moreover, the influence of structural orientation and shape factor on the magnetic and MCEs of RCuAl (R=Er, Tm) compounds has also been revealed.

**Keywords:** polycrystalline compound; the structural orientation; shape factor; magnetic; magnetocaloric effects

# POSTER Session 2

## Symposium J : Materials Characterization and in situ/3D/4D Analysis

**P-J0287** **Evaluation of irradiation induced hardness and microstructure of Zry-2 under applied stress**
Luwei Xue (Kyushu University, Japan)

**P-J0700** **Material Characterization of SiON films Deposited by PECVD for Thin Film Encapsulation of OLEDs**
Seokyoon Shin (Advanced Institute of Convergence Technology, Korea)

**P-J0826** **Correlation study of nonlinear ultrasonic parameters to steels weld microstructure**
Hyunmyung Kim (FAINDUS Co., Korea)

**P-J0878** **Microstructural effect on the resistance to fatigue crack growth of high-entropy alloys**
Wonhui Jo (Gyeongsang National University, Korea)

**P-J1048** **In-situ studies on microstructures and mechanical properties in metallic materials using pulsed neutron diffraction at TAKUMI**
Wu Gong (Japan Atomic Energy Agency, Japan)

**P-J1068** **Characterizing interfacial mechanical properties of post-heat treated Ti/Al clad materials**
In-Chul Choi (Kumoh National Institute of Technology, Korea)

| P-J0287 |

# Evaluation of irradiation induced hardness and microstructure of Zry-2 under applied stress

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## Abstract

Zircaloy-2 is located closest to the fuel in boiled water reactors as the fuel cladding tube. During reactor operation, fuel cladding tubes are affected by the stress due to UO2 pellet-cladding interactions. In this study, we investigated the microstructural evolution and hardening of Zircaloy-2 under irradiation with 3.2 MeV Ni3+ ions using TEM examination, nano-indentation measurements and energy-dispersive spectroscopy analysis. The materials were irradiated at different damage levels under applied stress.

The results show that <a> loops form at doses below 0.05 dpa, and the density saturates at around 0.1 dpa. The Orowan equation was used to calculate the contribution of <a> type dislocation loops to the hardening, and the calculated values were in good agreement with the experimental results, with the obstacle strength factor of <a> loops as 0.25.

At higher dose levels, <c> loops only nucleate above a threshold dose of 20 dpa at 400 ˚C. STEM observation reveals a decrease in hydride density and size in the irradiated region compared to the unirradiated region. Additionally, the dissolution of Fe atoms from Zr(Fe, Cr)2 precipitates due to irradiation was detected using EDS. However, Zr2(Fe, Ni) precipitates remained stable under the same irradiation conditions.

The effect of applied stress on the formation of dislocation loops was not obvious. The results confirmed that the <a> loops were mainly responsible for the hardening of the material under low-dose irradiation. Futhermore, the study discussed the effect of different conditions on the formation of <c> loops in the Zircaloy-2.

**Keywords:** Zirconium alloy; applied stress; ion irradiation; dislocation loop; energy-dispersive spectroscopy

| P-J0700 |

# Material Characterization of SiON films Deposited by PECVD for Thin Film Encapsulation of OLEDs

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## Abstract

Organic light-emitting diodes (OLEDs) require a passivation layer to protect the active layer from moisture and oxygen due to their vulnerability to these gases. Conventional glass-lid encapsulation is incompatible with flexible devices, so thin film encapsulation (TFE) has been extensively studied as an alternative method. For large-scale industrial production, plasma-enhanced chemical vapor deposition (PECVD) is more appropriate for preparing TFE films. The typical TFE barrier via PECVD is mainly composed of silica-based inorganic compounds. Among them, SiON has better barrier properties compared to SiOx and better photopermeability compared to SiNx. To develop high-quality TFE films, it is crucial to understand the fundamental degradation behavior of SiON due to moisture and oxygen.

In this study, we investigated the robustness mechanism in SiON films applied as TFE materials. The gases (SiH4, NH3, and N2O) used for PECVD were the same as those used for the conventional film, but their flow rates, process pressures, and powers were varied. Compared to the conventional film, the robust film exhibited an oxidation rate that was more than two times slower. During the heat-soak reliability test at 85°C/85% RH, it showed a different O-rich SiON interfacial layer formed from the SiON surface due to abnormal oxidation behavior caused by nano/micro-defects in the conventional film. This was attributed to the lower gas flow rate and longer mean free path in the deposition conditions for the robust film, resulting in a lower density of nano-defects and preventing abnormal oxidation behavior.

**Keywords:** SiON (Silicon Oxynitride), PECVD (Plasma-Enhanced Chemical Vapor Deposition), TFE (Thin film encapsulation), OLEDs (Organic Light-Emitting Diodes)

| P-J0826 |

# Correlation study of nonlinear ultrasonic parameters to steels weld microstructure

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## Abstract

Nonlinear ultrasonic testing (NUT) technique can be used to identify microscopic material properties over conventional (linear) UT owing to its high sensitivity in which the nonlinear parameters establish a set of signal pattern recognitions such as forming higher harmonic waves. In this study, laser welding process was applied to steel plates of SS400, SM45C, SUJ2, and SKD11 while microstructure observations of welded specimens were carried out. After careful selection of microstructure features, signals pattern processing algorithms were determined to identify the weld quality (such as inclusion formation). It was evident that the nonlinear parameters made a valid correlation to the weld microstructure as ultrasonic guided wave(UGW)-based diagnosis technique.

**Keywords:** Nonlinear ultrasonic, Steels, Laser weld, Ultrasonic Guided Wave(UGW), Signal processing algorithm

| P-J0878 |

# Microstructural effect on the resistance to fatigue crack growth of high-entropy alloys

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## Abstract

High-entropy alloys (HEA) has been found to display its superior damage tolerance achieved by the slip planarity and deformation twinning. In the fatigue crack growth (FCG) behavior, the tendency for slip reversibility, originating from a relatively large grain size, were contributed to a higher the threshold stress intensity factor range (ΔKth). In this study, FCG behavior of HEAs with different microstructure was studied under the load ratio of 0.1 at room temperature. Despite increase in grain size to 100 μm, the increment of ΔKth value is restricted compared to the specimen with smaller grain size (30 μm). ΔKth value of the LT specimen is higher than that of the TL specimen due to anisotropic direction of sub-grain structures. Therefore, a systematic study of the FCG behavior enabled to understand the microstructural dependence of ΔKth value in HEAs.

**Keywords:** High-entropy alloys; Fatigue crack growth; Threshold stress intensity factor; anisotropic

| P-J1048 |

# In-situ studies on microstructures and mechanical properties in metallic materials using pulsed neutron diffraction at TAKUMI

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## Abstract

Mechanical properties, as the principal properties of structural metallic materials, are governed by the microstructures. To track the structure-property relationship associated with various solid-solid reactions such as phase transformation and plastic deformation, is crucial for the development of structural metallic materials. TAKUMI [1], an engineering materials neutron diffractometer at MLF, J-PARC, covering a large d-range with a good balance between high neutron flux and high resolution is reliable to investigate various dynamic phenomena associated with microstructure evolution and deformation behavior. In addition, a variety of specifical sample environments at TAKUMI allow the in-situ studies under extreme environments such as cryogenic deformation (10K~), thermomechanical controlled process (~1473K), fatigue, etc. Crystallographic information including phase fraction, lattice strain (stress), texture, dislocation density, etc. as obtained by neutron diffraction can uniquely provide insights into microstructure evolution and deformation mechanisms in bulky materials. In the presentation, several recent studies on microstructure evolution and deformation mechanisms in metallic materials including steels, high-entropy alloys, magnesium alloys using in-situ neutron diffraction via TAKUMI will be introduced.

**Reference:**

[1] BL19 TAKUMI website: https://mlfinfo.jp/en/bl19/

**Keywords:** In-situ neutron diffraction; Deformation; Phase transformation; Metallic materials.

| P-J1068 |

# Characterizing interfacial mechanical properties of post-heat treated Ti/Al clad materials

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## Abstract

Titanium and titanium alloys are expensive and have poor room temperature formability, although they have low density, high specific strength and excellent corrosion resistance. Therefore, in order to reduce the cost and achieve excellent properties, titanium and titanium alloys are clad with aluminum and its alloys, which are inexpensive and have a low density and excellent formability at room temperature. Although cladding is a widely used solid-state joining technique, the post-heat treatment of clad materials is required to improve their interfacial properties, which is important to ensure the reliability of clad materials. Therefore, in this study, the relationship between the microstructure and mechanical properties at the interface of Ti/Al clad materials after post-heat treatment was analyzed. The thickness of the diffusion and intermetallic compound layer was increased with increasing the post-heat treatment due to the active diffusion of Al atoms. As a result, their uniaxial and nanomechanical properties were varied with the interfacial properties of the Ti/Al clad material.

**Keywords:** Cladding, Ti, Al, Interfacial property, Nanoindentation

# POSTER Session 2

## Symposium K : High-Entropy Materials and Amorphous Materials

**P-K0052** **The effect of initial microstructure on the cryogenic tensile behavior of a ferrous medium-entropy alloy**
Jiyeong Lee (Pohang University of Science And Technology, Korea)

**P-K0306** **Effect of Sintering Temperature on Microstructure of Zr-Cu System Glassy Alloy**
Shunsuke Kawasaki (National Institute of Technology, Kagoshima College, Japan)

**P-K0379** **Local structural changes during glass formation in Zr80Pt20 alloys**
Siyuan Zha (Waseda University, Japan)

**P-K0396** **Molecular dynamics study on the effects of multiple elements on grain boundary migration in high-entropy alloys**
Kohei Shiotani (Kanazawa University, Japan)

**P-K0399** **Local atomic structures and quasicrystal formation in Zr70Cu29Pt1 metallic glasses**
Kudo Shinya (Waseda University, Japan)

**P-K0502** **Crystallization Kinetics and Thermoplastic Forming Condition of TiCu-based bulk metallic glass**
Ki Buem Kim (Sejong Univercity, Korea)

**P-K1173** **Enhanced mechanical properties of Nb-Ta-V-Ti high entropy alloy with in-situ TiC particles**
Hyeok Jae Choi (Kongju National University, Korea)

**P-K1176** **Novel Zr-Ti-Ni-Cu metallic glass brazing fillers for joining Ti-6Al-4V alloy**
Jin Kyu Lee (Kongju National University, Korea)

| P-K0052 |

# The effect of initial microstructure on the cryogenic tensile behavior of a ferrous medium-entropy alloy

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## Abstract

In this study, a ferrous medium-entropy alloy (FeMEA), Co18.5Cr12Fe55Ni9Mo3.5C2 (at%), was subjected to annealing in the temperature range of 900 to 1200 °C. The influence of the presence or absence of precipitations and the difference in grain size on the cryogenic tensile deformation behavior was investigated. When precipitations were present, the alloy exhibited exceptional strength, with yield strength reaching ~1 GPa and ultimate tensile strength reaching ~1.8 GPa, along with elongation levels of approximately 20%. In the absence of precipitations within the heat treatment temperature range, a minor decrease in yield strength was observed, while an elongation exceeding 100% was achieved. The variation in composition due to the formation of precipitations and differences in grain size led to varying stability of FCC phases in different specimens. This, in turn, resulted in distinct BCC martensitic transformation kinetics and work hardening behavior due to deformation-induced phase changes

**Keywords:** Ferrous MEA, phase stability, precipitation hardening, DIMT

# Effect of Sintering Temperature on Microstructure of Zr-Cu System Glassy Alloy

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## Abstract

Metallic glasses (MGs) have attractive properties, such as high strength, low elastic modulus, high corrosion resistance, etc. However, most MGs are brittle and show the zero plastic deformation. Currently, MG matrix porous composites have the considerable promise as not only high strength but also ductile material. The objective of the study is to develop a MG matrix composite to enhance the plasticity of MG based material.

In the present study, powder metallurgy techniques, i.e., gas atomization (GA) and spark plasma sintering (SPS), were applied to fabricate the glassy and porous metallic materials.

Zr-Cu system alloys, which has high glass forming ability, were used. Alloy composition was Zr50Cu40Al10 (at.%). Effect of sintering temperature of SPS on the microstructure of sintered compact were investigated. Microstructures of fabricated materials were investigated by means of X-ray diffraction techniques. As the result, it was confirmed that the alloy powder and sintered compact with glassy microstructure can be obtained by GA and SPS process, respectively. Furthermore, it was found that the microstructure of sintered compacts varies with sintered temperature. Crystallization occurred at the high temperature SPS process.

**Keywords:** Metallic glasses, gas atomization, spark plasma sintering, sintered compacts, composite

| P-K0379 |

# Local structural changes during glass formation in Zr80Pt20 alloys

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## Abstract

The relationship between the local atomic arrangements and glass formation in metallic glasses has attracted the great attention of many researchers so far. Especially in Zr-based metallic glasses, it was revealed that icosahedral atomic clusters and their connections play an essential role in glass formation. In this study, we focused on a Zr80Pt20 metallic glass, including numerous icosahedral atomic clusters as local atomic arrangements. In the cooling process, the spatial distributions of icosahedral atomic clusters at various temperatures were investigated by molecular dynamics simulation. It was found that icosahedral atom clusters were formed with Pt atoms at the center, and the fraction was increased with decreasing temperature. We also traced specific Pt atoms to probe the dynamic behavior of atomic environments around them in the cooling process. As a result, it was clarified that atomic clusters were partially formed above the glass transition temperature and gradually changed into icosahedral shapes across the glass transition. Additionally, the persistence of icosahedral atomic clusters was also investigated in the isothermal relaxation process. Although a ratio of icosahedral atomic clusters to the whole structures remains almost unchanged, it was revealed that the lifetime for each icosahedron strongly depends on the relaxation temperature.

**Keywords:** metallic glass, amorphous, molecular dynamics simulation

| P-K0396 |

# Molecular dynamics study on the effects of multiple elements on grain boundary migration in high-entropy alloys

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## Abstract

High-entropy alloys (HEAs), which are solid solution materials obtained by mixing more than four elements with near-equimolar fractions, have been reported to exhibit higher resistance to grain boundary (GB) migration than conventional alloys such as binary dilute alloys. In binary dilute alloys, dynamic elemental segregation to GBs subsequent GB solute drag during its migration increases the force required for the GB migration. However, it remains unclear whether the mechanism for suppressing GB migration in HEAs is similar to the one in the dilute alloys, or newly appears due to containing multiple elements. In this study, to elucidate the mechanism for retarding GB migration in HEAs, we investigate the effects of the multiple elements in a HEA on GB migration by comparing with a binary alloy through molecular dynamics (MD) simulations and a classical GB migration theory proposed in binary alloys.

We find through MD simulations that the GB migration mechanism for the HEA can be almost the same as for the binary alloy, i.e., dynamic elemental segregation to GBs subsequent GB solute drag. However, applying the classical GB migration theory to the HEA shows only qualitative coincidence to the force required for GB migration obtained from the MD simulations. It indicates that containing multiple elements can be a key factor to realize high GB migration resistance in the HEA. Our study suggests that lattice distortion caused by a mixture of multiple elements can play a significant role not only in dislocation glide but also in GB migration.

**Keywords:** High-entropy alloys, Grain boundaries, Grain boundary migration, Elemental segregation, Solute drag

| P-K0399 |

# Local atomic structures and quasicrystal formation in $Zr_{70}Cu_{29}Pt_1$ metallic glasses

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## Abstract

The formation of quasicrystals from metallic glasses has been extensively investigated mainly in Zr-based metallic glass systems. Saida et al. reported that the nanoscale icosahedral quasicrystalline phase is formed by adding only 1 at.% of noble metals to Zr-Cu metallic glasses. In the present work, we focused on the addition of Pt and then examined the local atomic structures of glassy states and the subsequent quasicrystal formation in Zr70Cu29Pt1. The structure model of the glassy state was prepared by combining conventional and ab-initio molecular dynamics simulations. The binary Zr70Cu30 model was initially constructed using embedded atom model potentials, and 1 at.% of Cu atoms were then replaced with Pt atoms. Subsequently, the obtained ternary configuration was fully relaxed using the ab-initio calculation. It was revealed that coordination numbers for Pt atoms are gradually increased or almost unchanged during the relaxation process. Moreover, the Voronoi polyhedral analyses showed that the relaxation, especially at 500 K, leads to the formation of icosahedral or icosahedral-like atomic clusters. On the other hand, the quasicrystal formation was experimentally confirmed by using X-ray diffraction. By subtracting the diffraction peaks of the equilibrium Zr2Cu phase, some peaks originated from the icosahedral quasicrystal phase were confirmed using Rietveld analysis. The relationship between icosahedral atomic clusters and quasicrystal formation is also discussed.

**Keywords:** amorphous; metallic glass; quasicrystal; structure analysis

| P-K0502 |

# Crystallization Kinetics and Thermoplastic Forming Condition of TiCu-based bulk metallic glass

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## Abstract

Bulk metallic glasses (BMGs), noted for high glass forming ability and high thermal stability on the supercooled liquid, have been developed in various alloy systems. The BMGs also have exhibited superplastic-like deformation behavior resulting from the significant decrease of their viscosity in the supercooled liquid region (SLR). The superplastic-like properties on SLR facilitate the net-shape process using thermoplastic forming (TPF). For the TPF process, BMGs essentially need to good glass forming ability, low viscosity (fragile liquid) in the SLR, a low processing temperature and a long processing time before crystallization. In order to optimize TPF processing condition, the incubation time before crystallization and viscosity value depending on temperature within SLR are very important i.e., the thermoplastic formability strongly depends on processing temperature on SLR. Therefore, it is essential to understand the crystallization kinetics and evaluate viscosity for obtaining the optimal TPF processing condition of the BMGs.

In the present study, we investigated the crystallization kinetics of a monolithic TiCu-based BMG exposed at elevated temperatures within SLR. The as-cast BMG showed a relative large SLR (~ 70 K) during continuous heating. The incubation time for crystallization of the as-cast BMG was tested during isothermal annealing with different temperatures on SLR. The viscosity changes on SLR were measured by using thermo-mechanical analysis. Based on these analysis, a feasible TPF processing condition was determined by considering incubation time for crystallization and viscosity within SLR. In addition, a laboratory-scale TPF experiment was performed to evaluate thermoplastic formability of the BMG.

**Keywords:** Bulk metallic glass; Crystallization kinetics; Viscosity; Thermoplastic forming

| P-K1173 |

# Enhanced mechanical properties of Nb-Ta-V-Ti high entropy alloy with in-situ TiC particles

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## ABSTRACT

Refractory high entropy alloys (HEAs) are typically manufactured through vacuum arc melting due to the elevated melting points of their constituent elements. Nevertheless, as-cast refractory HEAs frequently exhibit coarse dendritic structures and segregation, resulting in undesirable mechanical properties. A promising method for achieving more uniform microstructures and enhancing mechanical properties entails employing mechanical alloying followed by consolidation processes.

This study investigates the influence of in-situ TiC particles on both the microstructure and mechanical properties of Nb-Ta-V-Ti High-Entropy Alloys (HEAs). The HEA matrix composites were fabricated through a two-step process, involving high-energy ball milling, followed by spark plasma sintering. Structural characterization was carried out using X-ray diffractometry (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Compressive strength measurements of the HEAs were conducted at both room temperature and elevated temperatures, employing a strain rate of 1x10-3s-1. The findings indicate that the in-situ TiC-reinforced Nb-Ta-V-Ti HEA exhibited a yield strength of 2100 MPa at room temperature and 1090 MPa at 800°C.

**KEYWORDS :** Refractory High entropy alloy, Composite material, Powder metallurgy, Mechanical alloying, Spark plasma sintering

| P-K1176 |

# Novel Zr-Ti-Ni-Cu metallic glass brazing fillers for joining Ti-6Al-4V alloy

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## Abstract

In the context of brazing in Ti-based alloys, the low melting temperature of the brazing filler metal plays a crucial role due to the α-β phase transformation. Zr-based metallic glasses have garnered significant attention as an efficient means of producing ribbon-shaped filler metals for brazing Ti and Ti-6Al-4V alloys using a melt-spinning process. Metallic glass fillers offer exceptional microstructure uniformity thanks to their amorphous atomic structure, with melting temperatures typically lower than those of conventional casting materials. Also, it is facilitated to make filler metal into foils due to the high workability of amorphous alloy. This study presents the development of Zr-Ti-Cu-Ni metallic glass fillers, produced through the melt spinning process, for brazing Ti-6Al-4V alloys. We also investigate the interfacial microstructure and mechanical properties of the brazed joints. The microstructure of the brazed joint was examined using scanning electron microscopy (SEM) coupled with Electron Probe Micro-Analysis (EPMA). Tensile tests were conducted at room temperature and a strain rate of 1x10-4s-1.

**Keywords:** metallic glass, ribbon, Ti alloy, brazing, filler

# POSTER Session 2

## Symposium L : Composite, Coating and Hetero-Materials

**P-L0828** **Study on corrosion resistance of carbon-based anti-corrosion coating in hot molten salt**
Wenjie Hou (Baowu Carbon Technology Co., Ltd, China)

**P-L0843** **Bonding Properties of Metal Matrix Composites through Brazing: Optimizing Parameters and Filler Material Composition**
Taeho Lee (Korea Institute of Material Science, Korea)

**P-L0864** **A study on the improvement of neutron absorption and thermal conductivity of aluminum matrix composites**
MINWOO KANG (Korea Institute of Materials Science, Korea)

**P-L0898** **Effect of improving mechanical properties according to the content of in-situ gamma prime phase in Ni-TiC-Ti2AlC MAX-phase MMC**
Minsu Kim (Korea Institute of Materials science, Korea)

**P-L1069** **Design and Toughening of High-performance Alloy Coatings and Heat-resistant Aluminum Alloys based on Theoretical Calculations**
Cai Jianming (Xi'an Jiaotong University, China)

| P-L0828 |

# Study on corrosion resistance of carbon-based anti-corrosion coating in hot molten salt

**Wenjie Hou**[1], Benjamin Grégoire[2], Shengze Yao[1], Weiyu Deng[2], Hongyi Zhao[1], Yulong Ding[2]

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## Abstract

The corrosion problem caused by hot molten salt in concentrating solar power (CSP) system is one of the problems that need to be solved urgently. The development of high temperature corrosion-resistant coatings is a key point to solve this problem. In this work, the protection of commercially available graphite paint GRAPHIT 33 coating and carbon-based slurry C coating on carbon steel A516 was evaluated in the environment of air, salt vapor and molten solar salt at 565°C. The results of comparative test and analysis show that the carbon-based slurry C coating can slow down the corrosion of A516 in 565°Csolar salt to a certain extent, and the formed corrosion layer is dense and continuous.

**Keywords:** carbon-based coatings; anticorrosion; high temperature molten salt.

| P-L0843 |

# Bonding Properties of Metal Matrix Composites through Brazing: Optimizing Parameters and Filler Material Composition

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## Abstract

Metal matrix composites (MMCs) are advanced materials that combine a ductile metal matrix with ceramic reinforcements, offering superior properties compared to single-component materials. The type and fraction of the reinforcement can be tailored to control the characteristics of composites. However, the practical application of MMCs in various industries requires effective post-processing techniques, including shaping and bonding.

Generally, soldering, brazing, and welding are used to join materials. Soldering, although conducted at lower temperatures, often results in weaker joint strength than other joint method. Welding can result in property degradation due to the high process temperatures, which impede control over matrix melting and reinforcement/matrix reactions. In contrast, brazing allows for joining at temperatures that preserve the integrity of the composite while promoting diffusion between the matrix and filler material. It means that this facilitates the formation of strong joints without compromising the properties of materials. These advantages of brazing are suitable and attractive method to apply for bonding each other of MMCs.

While extensive research exists on brazing for metal-to-metal joints, studies on brazing MMCs are relatively scarce. Therefore, this study is investigated optimizing the brazing parameters and filler material composition to enhance the bonding property of MMCs. The findings from this study will contribute to the development of effective post-processing techniques for MMCs, enabling their broader application in various industrial sectors.

**Keywords:** Brazing, microstructure, mechanical property, metal matrix composite

| P-L0864 |

# A study on the improvement of neutron absorption and thermal conductivity of aluminum matrix composites

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## Abstract

Metal matrix composites (MMCs) have many advantages in properties such as hardness, strength, wear and corrosion resistance, stiffness and so on. These superior properties of MMCs can be possible to apply for the extreme environment materials. As an example of the extreme environment application, aluminum matrix composites (AMCs) incorporating boron carbide(B4C) have been developed and used as neutron absorbing materials (NAMs) in transportation baskets, storage racks, and storage casks for spent nuclear fuel (SNF).

SNF emits not only thermal neutrons but also high levels of heat. Therefore, it is important to enhance thermal properties of NAMs for applying those to materials of the storage of SNF. However, previously developed NAMs have been suffered from low thermal conductivity due to the high content of reinforcements with low thermal conductivity. This issue needs to be solved.

For enhancing the properties of the AMCs used in NAMs, in this study, the neutron absorption and thermal properties of the AMCs was improved by controlling interfacial characteristics and hybridization of reinforcements.

**Keywords:** Aluminum, metal matrix composite, neutron absorber, spent nuclear fuel, thermal conductivity

| P-L0898 |

# Effect of improving mechanical properties according to the content of in-situ gamma prime phase in Ni-TiC-$Ti_2AlC$ MAX-phase MMC

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## Abstract

For decades, Metal Matrix Composites (MMCs) have been recognized for their superior strength, stiffness, wear resistance, oxidation resistance, thermal stability and low density compared to conventional alloys. In particular, due to its excellent thermal stability in cryogenic and high-temperature environments such as aerospace, military, energy storage, and energy generation, it is being studied as a material to replace existing alloy materials.

MMC, which is mainly studied in harsh environments, is a composite material with a matrix of Ni-base superalloy, which has excellent thermal stability even at high temperatures such as Inconel, and has superior mechanical properties. Ni-base superalloy is a material that secures high-temperature strength by depositing γ' or γ''-phase, which is a strengthening phase that shows excellent physical properties even at high temperatures, in the matrix. γ' in the matrix of MMC, which is reported to be beneficial for high-temperature strength. When the phase exists, it is believed that higher high-temperature strength can be obtained than the existing Ni-base superalloy.

Therefore, in this study, the precipitation amount of γ'-phase was varied in TiC-reinforced MMC to obtain a composite material of γ'-phase. In order to examine the effect on high-temperature strength, Al, an element of the γ' phase, was employed in different amounts through Ti2AlC MAX-phase inside the TiC-Ni composite material. The relationship between the amount of γ'-phase production and the effect of the γ'-phase content on the high-temperature strength of TiC-Ni MMC were studied.

**Keywords:** Metal Matrix Composites(MMCs), Ni-base superalloy, MAX-phase, gamma prime phase, high temperature strength.

| P-L1069 |

# Design and Toughening of High-performance Alloy Coatings and Heat-resistant Aluminum Alloys based on Theoretical Calculations

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**Abstract:**

During the process of alloy material fabrication using magnetron sputtering, the system deviates from equilibrium and easily obtains metastable phases. By combining computational methods such as CALPHAD with experimental techniques, a phase diagram of metastable phases can be constructed for the system, allowing for the investigation of the influence of chemical composition and fabrication processes on material structure, and subsequently evaluating the performance of materials under different structures. For instance, a ternary aluminum-based metastable phase diagram constructed based on CALPHAD and key experiments is used to describe the phase formation behavior of commonly used hard coating material Al-Ti-N in industrial production. Similarly, the construction of a thermodynamic database for the Al-Mn-X system facilitates the understanding of the influence of chemical composition on phase formation in the alloy, thereby providing theoretical guidance for the development of high-strength and tough Al-Mn-based nano-dual phase alloys. This project envisions expanding existing research methods by integrating theoretical calculations, experimental fabrication, electrochemical testing, and advanced characterization techniques to efficiently establish the correlation between composition, structure, and mechanical properties in the Al-Mn system, ultimately leading to the fabrication of high-strength and tough Al-Mn-X alloys.

**Keywords:** magnetron sputtering; nano-dual phase; metastable state; thermodynamic calculation

# POSTER Session 2

## Symposium N : Computational Materials and Artificial Intelligence

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Zhangcan Yang (Huazhong University of Science And Technology, China)

| P-N0144 |

# A study on estimation of changes in mechanical material properties accroding to changes in pore shape using Representative Volume Element method

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## Abstract

Recently, there has been an increasing demand for various materials that secure high performance, such as composites that have excellent mechanical properties. In particular, electrodes used in the battery industry have pores, and porosity should be considered when conducting structural analysis simulations for their manufacture. Because there is a difference in mechanical properties between materials with and without pores, various studies are being conducted to analyze this. Many studies are being conducted to derive representative mechanical properties based on homogenization method. In particular, many studies use the RVE(Representative Volume Element) method due to its ease of application and high consistency. In this study, changes in material properties were studied using RVE when the shape of pores was altered in materials.

**Keywords:** Representative mechanical properties, Porosity, Shape of pores, Finite element method, Representative volume element

| P-N0260 |

# A deep learning based surrogate model in design optimization of aluminium frames for large-scale photovoltaic modules

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## Abstract

AI-based surrogate models are being continuously researched as an alternative to reduce the physical time required for finite element analysis by using statistically-based models with relatively lower computational requirements to predict results with high fidelity, thus mimicking the results of finite element analysis at a lower cost. Meanwhile, the development of module integration with large-area solar cells is progressing worldwide to meet the demand for high-output modules as the size of wafers used in solar cell manufacturing increases, and the size of modules is also increasing. However, as the size of the solar modules increases, their weight increases as well, and applying the existing aluminium frame may result in deflection due to self-weight and external pressure. If the cells are deformed due to the load, internal cracks and damage may increase dead cells, which leads to a decrease in charge rate and efficiency. Therefore, in this study, we aimed to design an aluminium frame with minimal deflection by applying an alternative AI-based surrogate model and changing the shape of the frame for large-scale modules. Firstly, the existing commercial aluminium frame was applied to conduct finite element analysis by applying self-weight, wind pressure, and snow load to 585W M10-cell solar module and analyzing the deflection amount. Afterwards, surrogate model that can mimic the analysis results by learning from the finite element analysis was created using AI, and an aluminium frame that minimizes the deflection of the module under the applied load was designed using the created surrogate model.

**Keywords:** Deep leaning, Surrogate model, Finite element analysis, Photovoltaic modules, Aluminium frame

| P-N0282 |

# Systematic evaluation of segregation band formation using t he MPF-LB simulation of semi-solid simple shear deformation

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## Abstract

Semi-solid deformation occurs during a casting process where a solid–liquid coexistence region is deformed by gravity, convection, external force, and so on. During this process, solidification defects such as segregation bands form because of the interaction and rearrangement of grains, and therefore, the detailed evaluations of semi-solid deformation phenomena are necessary. A shear band with a high liquid fraction was observed in the rotating experiment of a cross-shaped blade in a solid–liquid coexistence system and shear deformation of semi-solid material [Nature 445 (2007) 70-73]. However, systematically evaluating factors that characterize semi-solid deformation (such as solid fraction and grain size) is difficult by changing evaluating factors accurately using experimental methods.

In this study, we reproduced semi-solid simple shear deformation using a multi-phase-field lattice Boltzmann (MPF-LB) model developed to express polycrystal solidification with liquid flow and crystal motion [Comp. Mater. Sci. 197 (2021) 110658]. Further, we quantified the semi-solid deformation by systematically changing the solid fraction, grain morphology, grain size, grain arrangement, deformation rate, and so on. The results of this study will improve the accuracy of the one-dimensional semi-solid deformation model [IOP Conf. Ser. Mater. Sci. Eng. 84 (2015) 012011] and contribute to the efficient prediction of the segregation band.

**Keywords:** Phase-field method, Lattice Boltzmann method, Semi-solid deformation, Segregation band.

| P-N0448 |

# Many-body effects on glass formation in molecular dynamics simulation

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## Abstract

The embedded atom model (EAM) potentials that take the effect of multiple surrounding atoms into consideration have been widely used for molecular dynamics simulations for defects, surfaces, and disordered structures. The many-body effect should play an essential role in disordered structures such as liquids or glasses, because each atomic site possibly has a different coordination number. To confirm this, we conducted the simulation of glass formations for a monoatomic Cu system using two-body and EAM potentials. The faster cooling with a cooling rate of 1.0 x 1014 K s-1 led to the formation of glassy states for both cases. On the other hand, some crystals were formed in the model made by the two-body potentials during the slower cooling of 1.0 x 1012 K s-1, although the model made by EAM potentials retained a disordered structure. In the glassy structure obtained by the two-body potentials, there are a lot of crystal-like (fcc like) atomic clusters indexed by <0 4 8 0> and <0 5 4 3>, which are hardly found in the EAM model. In contrast, there is an abundance of icosahedral or icosahedral-like atomic clusters such as <0 0 12 0> and <0 2 8 1> in the model by the EAM potentials. Therefore, it is plausible that the formation of icosahedral atomic clusters instead of crystal-like clusters should be critical for the glass formation. The many-body effects on the formation of icosahedra are also discussed.

**Keywords:** Metallic glass, Atomic structure, Glass forming ability, Molecular dynamics and

Poster Session 2

| P-N0688 |

# Molecular dynamics simulation of solidification microstructure formation under large temperature gradient

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## Abstract

Melting and solidification under a very large temperature gradient (super temperature field) under additive manufacturing (AM) is very different from the normal temperature field, and microstructure control in the super temperature field is important for establishing high-precision 3D printing technology. Although there are examples of phase-field simulations for understanding solidification and microstructure formation in super temperature fields [1], molecular dynamics (MD) simulations are not commonly used to understand microstructure formation on an atomic scale due to the limitations of spatial scales. Recent improvements in computer performance have dramatically increased the spatial scales that can be analyzed by MD. Therefore, the objective of this study is to understand the solidification and microstructure formation processes at the atomic scale in a super temperature field using MD simulations. A solid-liquid coexistence model with a convex interface consisting of one million atoms was created, and the solidification process under various temperature gradients was investigated. Calculations with a negative temperature gradient confirmed the growth of a convex interface.

[1] M. Ohno, et al. Mater. Trans. 60 (2019) 170.

**Keywords:** Molecular dynamics simulation; Solidification; Large temperature gradient; additive manu

| P-N0689 |

# High-precision prediction of physical properties of molecular dynamic simulation using graph neural networks

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## Abstract

Graph convolutional network (GCN)-based machine learning (ML) models have been developed to predict the physical properties of metallic materials from graphical representations of atomic configurations in molecular dynamics (MD) simulations. The ML model, which combines GraphSAGE, a method derived from GCN, and simple perceptron, successfully predicts the temporal variation of potential energy in solid-liquid two-phase systems of metallic materials. The trained ML model was able to make good predictions for the characteristics of the training data. Furthermore, despite the lack of interatomic distance information in the graph representation, the model was able to make adequate predictions for unknown graph structures, confirming that its generalization performance is adequate. The significance of this study is that it shows that the graphical representation can be a good notation for predicting various properties from MD simulations, especially for large systems of metallic materials, since there is no established notation for atomic arrangements in MD simulations.

**Keywords:** Molecular dynamics; Machine learning; Graph neural networks; Graph representation; Solid-liquid coexisting system

| P-N0928 |

# Exploring austenite grain growth mechanisms in alloy steel during reheating using XAI

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## Abstract

Austenite-grain growth plays a crucial role in heat treatments, such as annealing and normalizing, as it directly affects the microstructures and overall properties of alloy steels. While empirical equations have been proposed for predicting austenite-grain growth during reheating, there is a need to improve prediction accuracy and analyse the underlying mechanisms and variable importance. Machine learning models offer a promising approach to enhance prediction accuracy without the need for additional experiments. In this study, we leveraged the power of explainable artificial intelligence (XAI) within machine learning models to predict austenite-grain growth with improved accuracy and explore variable importance and model mechanisms. A dataset comprising 458 usable data points was collected from the literature, followed by outlier analysis and removal using a boxplot. Hyperparameters are optimized using five-fold cross-validation and a grid search approach. Random forest regression (RFR) was selected as the preferred model based on its accuracy. To validate the enhanced accuracy of the RFR model, a comparison was made with an empirical equation. Furthermore, the SHAP analysis of XAI technique is employed to investigate the variable importance and mechanisms of the machine learning model.

**Keywords:** Alloy steel, Heat treatment, Austenite-grain growth, Explainable artificial intelligence(XAI), Machine learning

| P-N0935 |

# Prediction of cementite precipitation in austenite of low-alloy steels using XAI

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## Abstract

This study presents a machine learning model to predict the $\gamma/(\gamma + \theta)$ transformation temperature, which is also known as the Acm temperature in the FeC phase diagram. From the literature, 25,920 usable data points are collected, and the dataset is analyzed using a boxplot. The hyperparameters of the machine learning models are adjusted using fivefold cross-validation and grid-search techniques. An artificial neural network (ANN) model is selected based on the determination coefficient. The ANN model is compared with an empirical equation to verify the improvement in the accuracy of the model. The significance of the variables was analyzed using the Shapley additive explanations method. Further, the variable prediction mechanisms are discussed.

**Keywords:** Machine learning; Cementite precipitation; Shapley additive explanations(SHAP); Prediction mechanism; Explainable artificial intelligence(XAI)

| P-N0948 |

# Tempered martensite hardness prediction and feature analysis using XAI in low-alloy steels

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## Abstract

Control of the mechanical properties through heat treatment in low-alloy steels is important to meet the requirements in the industrial fields. Several studies have been conducted to predict tempered martensite hardness according to the heat treatment process and composition of low-alloy steel through thermodynamic calculations and empirical equation. Although the effect of each variable value can be known to some extent from the empirical equation, it is difficult to analyse the overall effect of the variables and the effect of changes in each variable. In order to solve this problem, we proposed four machine learning algorithms to predict the hardness of low-alloy steels under various tempering conditions. More than experimental 1900 data were collected from the relevant literature for low-alloy steels. The RFR (Random forest regression) model with the highest accuracy was selected and compared with the existing equation. In addition, SHAP was used to confirm the average influence of variables on hardness. As a result, we analysed the exact average prediction mechanism and proposed the importance of the heat treatment process variable and composition of low-alloy steels.

**Keywords:** Low-alloy steels, Tempered martensite, Hardness, Machine learning, Explainable artificial intelligence (XAI)

| P-N1008 |

# Enhancement of the growth of a helium bubble through the strain field generated by itself

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## Abstract

As plasma facing materials of magnetic confinement fusion reactor, tungsten will be exposed to low-energy high-flux helium plasma, leading to the formation of subsurface helium bubbles and surface damage. Over-pressurized helium bubbles can induce large strain fields around the bubble, affecting the diffusion behaviour of helium atoms. In this study, the diffusion of helium atoms in strain fields is systematically investigated using molecular dynamics (MD) methods. Since a strain field can be seen as a combination of a uniaxial strain and a strain gradient, the effects of these two components are studied separately.

The results show that a uniaxial compressive strain can promote He diffusion in the direction of the compressive strain, while inhibiting He diffusion in the direction perpendicular to the compressive strain. The results also show that there is a drift diffusion for He along the direction of a decreasing stress gradient. The diffusion of helium atoms in the strain gradient follows the Einstein relation.

Our results reveal that a helium bubble can interact with free helium atoms through the strain field generated by itself. The bubble can attract helium atoms in the <100> directions, resulting in a significant increase of helium diffusion towards the bubble and an enhancement of the bubble growth. As a result, we suggest to use an effective capture radius of helium bubbles to account for this strain effect in higher scale simulations such as kinetic Monte Carlo or cluster dynamics.

**Keywords:** plasma facing materials; tungsten; helium bubbles; molecular dynamics; strain

Poster Session 2

# POSTER Session 2

## Symposium O : Materials for Sustainability (Green Steel, Recycling, and Corrosion)

**P-O0017** **Upgrade of instrument control system of Lean Oil Sealed Gasholder**
Quan Wang (Energy and Environment Management Center Of Angang Steel Co., Ltd., China)

**P-O0481** **Preparation of High-Purity Nickel by Floating Zone Refining under Hydrogen Atmosphere**
YuBo Wang (Kunming University of Science And Technology, China)

**P-O0504** **Color Transition Behavior of Cu-5Al-5Zn-1Sn Alloy with Low Stacking Fault Energy by Tailoring Grain Boundary**
Ki Buem Kim (Sejong Univercity, Korea)

**P-O0589** **Electrorefining of Ti in LiCl-KCl-NaCl-TiCl2 molten salt with oxygen concentration in CuTi feedstock**
KyuSeok Lim (Chungnam National University, Korea)

**P-O0594** **Inert anode-based eco-friendly electroreduction of magnetite**
Wooseok Choi (Chungnam National University, Korea)

**P-O0606** **Investigation of Inert Anode Materials for Carbon-free electroreduction of CaO**
WanBae Kim (Chungnam National University, Korea)

**P-O0612** **Improvement of Anode Charge/Discharge Performance through Ag and Li Alloying**
Seungho Lee (Chungnam National University, Korea)

**P-O0624** **Development of eco-friendly electroreduction method for producing Nd-Fe alloy from Nd2O3**
Donghee Lee (Chungnam National University, Korea)

**P-O0772** **Molten salt electrolysis of secondary resources and vacuum distillation for producing high-purity magnesium metal**
Hyeong-Jun Jeoung (Seoul National University, Korea)

**P-O0957** **Researching the feasibility of the binder remove and solvent recycle process through the use of green solvents for direct recycling of used batteries**
Cheol Kang (Korea Battery Industry Association, Korea)

**P-O1019** **Optimization of the discharge process of spent Li-ion batteries from electric vehicles for direct recycling**

Hyunseok Lee (Korea Battery Industry Association, Korea)

**P-O1020** **Causes of Capacity Fade in Lithium-Ion Batteries and Research on Direct Recycling**

Min-Ho Kim (Korea Battery Industry Association, Korea)

| P-O0017 |

# Upgrade of instrument control system of Lean Oil Sealed Gasholder

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## Abstract

Lean oil sealed gasholder is widely used for storaging blast furnace gas high or coke oven gas in iron and steel enterprises because of its many advantages. In order to ensure safety and environmental protection, the instrument system of 3 lean oil sealed gasholders which had been put into operation for 16 years has been reformed in the pressurized operation area of the gas branch of Angang Steel Co., Ltd. Energy and Environment Management Center. In this paper, the hardware configuration, grid structure and communication protocol of instrument control system of lean oil sealed gasholders are briefly introduced.

**Keywords:** configuration, structure, configuration

| P-O0481 |

# Preparation of High-Purity Nickel by Floating Zone Refining under Hydrogen Atmosphere

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## Abstract

This study focuses on preparing high-purity nickel using floating zone refining under hydrogen atmosphere to overcome challenges related to impurity removal. The utilized high-vacuum floating zone refining device minimizes contamination and external impurities. The purification process's effectiveness is particularly notable for gaseous impurities, such as carbon and oxygen, with removal rates reaching 94.5% and 96.3%, respectively. The purification mechanism involves hydrogen atoms reacting with gaseous impurities to form gaseous hydrides and bubble formation, contributing to the removal of impurities by adsorbing inclusions on the bubble surface.

**Keywords:** Nickel, Floating Zone Refining, Hydrogen Atmosphere, Bubbles, Removal Rate

| P-O0504 |

# Color Transition Behavior of Cu-5Al-5Zn-1Sn Alloy with Low Stacking Fault Energy by Tailoring Grain Boundary

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## Abstract

The color alloys have been studied for realization the alloy having own unique color. Manufacturing processes of colored layer on the surface of metals have the limitation of base material selection, and colored layer can be faded by mechanical and chemical damage. Thus, industrial field of metallic material have developed the color alloy. The Nordic Gold color alloy which has alloy composition of Cu-5Al-5Zn-1Sn exhibit novel color and remarkable properties. The single-phase colors alloy such as Nordic gold alloy are controlled the optical and mechanical properties by the control of density of state (DOS) and optical transition energy. However, this method has limitation that the area of property control is possible within the solid solubility limit. Therefore, the new strategy of optical property control has been studied. Cu-5Al-5Zn-1Sn alloy with low stacking fault energy (SFE) can be modified the microstructure by severe plastic deformation (SPD). When the low SFE alloys applied the SPD, the sliding of dislocation is restricted. Thus, the partial dislocation causes the deformation twin and nanocrystalline. These alloys also exhibit the specific grain boundary (Σ3 grain boundary) structure that possess the annealing twin. In the previous study, it is reported that the grain boundary energy can be affected to DOS.

In the present study, we investigated the color transition behavior of Cu-5Al-5Zn-1Sn alloy. As casting bulk alloy was conducted solid solution treatment at 700°C 30 minutes. The rolling was conducted from 6mm to 1mm thickness for generation of high density of grain boundary and dislocation. The annealing of samples was performed at 550°C 12 hours, 550°C 24 hours and 600°C 72 hours for recrystallization and grain growth. These samples were analysed microstructure and optical properties to establish the correlation of between the grain boundary energy and optical properties.

**Keywords:** Color alloy; Cu-Al-Zn-Sn alloy; grain boundary; Stacking fault energy; optical transition energy

| P-O0589 |

# Electrorefining of Ti in LiCl-KCl-NaCl-$TiCl_2$ molten salt with oxygen concentration in CuTi feedstock

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## Abstract

Titanium is a metal that is used as a core material in high-tech industries that require high strength and light weight, such as aerospace, national defences, and automobiles, because of its excellent characteristics of high specific strength and corrosion resistance. However, currently, most of the titanium materials in Korea are dependent on imports, and research on manufacturing titanium by reducing ilmenite and rutile, which are titanium oxides, is being actively conducted. In this study, the effect of the anodic dissolution rate according to the oxygen concentration in the anode feedstock was studied. TiO2 (Rutile) containing V, Zr, Fe, Al, and Si impurities was used to manufacture Ti metal having an oxygen concentration of 5 wt% using SHS (Self-propagating high-temperature synthesis) method. This was reduced with Mg at 1473K to produce CuTi alloys with various oxygen concentrations, and a study was conducted to selectively recover titanium from the prepared alloy. As the electrolyte, LiCl-NaCl-KCl molten salt of eutectic composition was used, and 7.5 mol% TiCl2 was added. In order to confirm the electrochemical behavior of titanium, cyclic voltammetry and anodic polarization analysis were performed. Ti and the anode recovered by electrorefining at a temperature of 500 ° C were analyzed for shape and concentration of impurities using FE-SEM and EDS, and the concentration of impurities in the molten salt was confirmed by ICP analysis.

**Keywords:** electrorefining, thermal reduction, titanium,

| P-O0594 |

# Inert anode-based eco-friendly electroreduction of magnetite

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## Abstract

Recently, global attention has been increasing towards climate change and other abnormal weather phenomena occurring worldwide. As a result, there is a growing trend of voluntary participation by global companies, such as RE100, to reduce carbon emissions. Consequently, efforts to reduce carbon emissions are being demanded across various industries, including the steel industry, which is actively conducting research to achieve carbon emission reduction.

While the steel industry has been researching reduction through hydrogen utilization, this paper focuses on the study of magnetite reduction using the well-known FFC (Fray-Farthing-Chen) process, which utilizes molten salt electrolysis. If the electricity required for hydrogen production is directly used for the reduction reaction of magnetite, an increase in energy efficiency is expected. In addition, magnetite has sufficient electronic conductivity and is suitable for electrolytic reduction. The FFC process involves the movement of oxygen ions from the oxide at the cathode to react with the graphite anode, generating COx, making it less environmentally friendly. Therefore, this study aimed to investigate the electroreduction process that generates oxygen using an inert anode as a replacement for the conventional graphite anode. In this study, electroreduction with an inert anode was performed to explore the environmentally friendly aspect of oxygen generation.

**Keywords:** Inert anode, Eco-friendly, Electroreduction, molten salt

| P-O0606 |

# Investigation of Inert Anode Materials for Carbon-free electroreduction of CaO

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## Abstract

The global implementation of carbon reduction policies has necessitated a need for transformation within various industrial sectors, particularly in carbon-intensive industries such as traditional metal manufacturing. Processes involving the use of graphite anodes in electrolytic metal production or the utilization of cokes or carbon-based substances in intermediate processing inevitably result in the emission of greenhouse gases such as CO2 and CO. In order to suppress this, it is necessary to replace the graphite anode with an inert anode.

In this study, we focused on the exploration of various inert anode materials. Initially, we employed deep learning techniques utilizing the material property database of the "Material Project" to classify materials based on characteristics such as electrical conductivity (Band gap) and thermodynamic stability (Formation E, Energy Above Hull)

Subsequently, a series of preliminary material evaluations is conducted to assess the suitability of the identified candidates for electroreduction. These evaluations encompass an in-depth analysis of material properties, considering factors such as electrical conductivity, anode dissolution behavior through anodic polarization analysis, stability under CaCl2-NaCl-CaO molten salt electrolytic conditions and overall performance as inert anodes. The final objective of this study is to present an efficient screening method for various inert anode materials and to identify materials with commercial feasibility within the carbon-intensive industry through verification evaluation.

**Keywords:** Inert anode, molten salt, electrolysis, carbon-free

# Improvement of Anode Charge/Discharge Performance through Ag and Li Alloying

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## Abstract

Currently available commercial secondary batteries commonly use cathode materials like LFP and NCM622. In this case, when the theoretical capacity expressed by the cathode material used is about 200mAh/g and when using a graphite anode with a theoretical capacity of about 300mAh/g, performance limitations of the secondary battery originate from the low-capacity cathode material [2]. However, considering high-nickel NCM cathodes, research is underway to address the performance limitations of secondary batteries caused by graphite anodes. Various alternative anodes are being investigated to achieve a high theoretical capacity, low reaction voltage, and high energy density. One promising candidate is Ag due to its lithiophilic properties, high electrical conductivity, and excellent mechanical stability. Therefore, in this study, we explore the electrochemical behavior of lithium ions in Ag by employing micro/nano-sized Ag powder in conjunction with graphite (Ag/C) as anode materials. The Ag/C composition is adjusted by increasing the proportion of graphite relative to Ag. Then, we confirm the performance of Ag/C anode and analyze the morphology and phase analysis by SEM, EDS and XRD.

**Keywords:** Electrochemical behavior, Anode, Li, Ag, Ag/C

| P-O0624 |

# Development of eco-friendly electroreduction method for producing Nd-Fe alloy from $Nd_2O_3$

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In commercial processes for neodymium production, graphite electrodes are commonly used, resulting in the generation of greenhouse gases such as CO, CO2 and PFC. To solve this issue, In the case of the Al smelting industry, eco-friendliness using inert anodes is underway. Inert anode maintains electronic conductivity in an oxidizing atmosphere of high-temperature molten salt and guarantees high chemical stability, so it is a material that can oxidize oxygen ions and generate only pure oxygen. In this study, the possibility of using inert anodes in the Nd electroreduction process was examined.

Measurement of basic electrochemical data was investigated to produce Nd-Fe alloy using Neodymium oxide (Nd2O3). Electrolysis of Nd2O3 was carried out using iron cathode (Fe) in a Lithium fluoride (LiF) - Neodymium fluoride (NdF3) molten salt at 1173 or 1123 K. To mitigate the significant time required for Nd3+ ions to react with Nd metal and convert the electrolyte to NdF2, Nd metal was added to NdF3, and experiments were conducted. The formation of NdF2 was measured using square wave voltammetry, and in addition, chronopotentiometry and basic electrochemical data were also measured. After electrolysis, the dissolution of the anodic constituents in the molten salt was measured and analyzed over time using ICP (Inductively Coupled Plasma) to predict the anode lifespan and evaluate the commercial viability. The penetration of the molten salt and changes in the formation behavior of the reaction layer were assessed using SEM/EDS (Scanning Electron Microscopy/Energy-Dispersive X-ray Spectroscopy).

**Keyworld :** Nd2O3, Electrolysis, NdF2, Square wave voltammetry

| P-O0772 |

# Molten salt electrolysis of secondary resources and vacuum distillation for producing high-purity magnesium metal

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## Abstract

To develop a green and novel Mg production process, molten salt electrolysis of secondary resources using a metal cathode, followed by vacuum distillation, was investigated. The electrolysis of ferronickel slag, aged ferronickel slag, and oxidized MgO-C refractory brick was conducted using a Cu cathode and C anode in MgF2 – LiF – KCl molten salt at 1043 K by applying an average current of 1.44 A in an Ar gas atmosphere. The average cell voltages were in the range of 2.48 – 2.75 V, and a mixture of MgCu2 and Cu (Mg) was obtained by the electrodeposition of Mg on the Cu cathode. Under a certain condition, the current efficiency was 92.3 %. Through vacuum distillation of the Mg alloys obtained at 1300 K, Mg metal with a purity of above 99.994 % was obtained. Therefore, it was demonstrated that a combination of molten salt electrolysis using a Cu cathode and vacuum distillation is feasible for producing high-purity Mg metal from secondary resources.

**Keywords:** Magnesium metal, secondary resources, electrolysis, copper cathode, vacuum distillation

| P-O0957 |

# Researching the feasibility of the binder remove and solvent recycle process through the use of green solvents for direct recycling of used batteries

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## Abstract

Recycle of after use batteries, usually, that shredded and then black mass or black powder is recovered, and valuable metals are recovered from the obtained powder through Pyrometallurgy or Hydrometallurgy.
This traditional method required to high-temperature equipment and the resulting carbon dioxide and a lot of industrial waste. In order to achieve low-carbon renewable energy and reduce industrial wastes, that obstacles must be overcome.

In this study, we chose the method of direct recycling and studied the recovery of black powder through direct recycling with SoH (State of Health) 90 % and 66 % real samples of after use batteries.
Furthermore, using a solvent (TEP) known as green solvent, we studied the possibility of direct recycling of used batteries through an approach that can be said to be more environmentally friendly than traditional methods.

Put TEP (triethylphosphate) in a beaker, heat and stirred at about 200 ° C and then insert an cathode cut into 2 cm X 2 cm. After stirring vigorously for about 3 hours and centrifuging at 8000 rpm for 15 minutes, the supernatant was separated, distilled water was added thereto, and PVDF and the conductive material were extracted and separated using the NIPS (non-solvent phase inversion separation) method.

Then, distilled water and the solvent were separated through the evaporation rotational concentration step, and then the solvent was evaporated and recovered to obtain a disk-shaped film.
FT-IR, XRD, and TGA analysis were performed to analyse the components of the disk-shaped film. Through this, it was confirmed that the components were pvdf and a conductive material.
As a result, the development of a process for removing impurities (binder and conductive material) in the direct recycling method of used batteries through the rotary evaporation step and the possibility of recycling the solvent through the recovery of the solvent used in this process were confirmed.
Through the above results, the possibility of an eco-friendly process was confirmed through the recovery of the solvent as well as the recovery of the black powder containing low impurities.

**Keyword :** Lithium Ion Battery recycling, After use battery recycling, Direct recycling, Black powder, Binder remove

| P-O1019 |

# Optimization of the discharge process of spent Li-ion batteries from electric vehicles for direct recycling

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## Abstract

Numerous studies on spent lithium-ion batteries (LIBs) recycled from electric vehicles have been conducted. However, research on preprocessing techniques to safely disassemble spent LIB packs has mainly focused on water-based discharge methods, such as salt-water discharge. However, salt-water discharge corrodes electrodes and the case, which results in internal contamination. Therefore, we conducted electrical discharge, which is suitable for the direct recycling process. We recovered spent LIBs from electric vehicles that were scrapped after operation and electrically discharged them to different voltages. As a spent LIB with a state-of-health of 66.8% was over-discharged, swelling increased, and even after being discharged to 0 V, the voltage could recover to 2.689 V. We analyzed the discharged spent LIBs through X-ray diffraction, scanning electron microscopy, and electrochemical impedance spectroscopy, and confirmed that the appropriate voltage is 2.5 V. The proposed electrical discharge process will be suitable for the direct recycling of spent LIBs in the form of pouch cells.

**Keywords :** Lithium ion battery, electric vehicles, spent Li-ion batteries, direct recycling

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| P-O1020 |

# Causes of Capacity Fade in Lithium-Ion Batteries and Research on Direct Recycling

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## Abstract

Lithium-ion batteries (LIBs) have revolutionized the field of energy storage, powering various applications ranging from portable electronics to electric vehicles. However, capacity fade, which refers to the gradual loss of battery capacity over cycling, remains a critical issue that hampers their long-term performance and reliability. This paper presents an overview of the causes of capacity fade in LIBs and explores the potential of direct recycling as an effective approach for sustainable battery management.

To address the challenges posed by capacity fade and promote sustainable battery management, direct recycling has emerged as a promising solution. Direct recycling involves the recovery and reuse of valuable materials from spent batteries to produce new battery components. This approach offers several advantages, including resource conservation, reduced environmental impact, and cost savings. However, successful direct recycling requires efficient methods for material recovery, purification, and reintroduction into the manufacturing process, as well as addressing potential performance limitations in recycled batteries.

This paper reviews recent research advancements in understanding the causes of capacity fade in LIBs and highlights the progress made in the field of direct recycling. It discusses various strategies to mitigate capacity fade, such as electrode/electrolyte interface engineering, electrolyte formulation optimization, and innovative recycling techniques. Further research is needed to develop robust and scalable recycling technologies and improve the overall sustainability of LIBs.

**Keywords:** Lithium-ion batteries, capacity fade, direct recycling, solid-electrolyte interface, sustainable battery management.

**Keywords :** Lithium ion battery, electric vehicles, spent Li-ion batteries, direct recycling

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