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2012 Fall Conference Abstracts

2012년도 대한금속·재료학회 추계 학술대회

초 록 집

■날짜 : 2012년 10월 25일(목)~26일(금)

■장소 : 창원컨벤션센터

■주최 : (사)대한금속·재료학회

■후원 : • 한국과학기술단체총연합회
• 경상남도
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KIM 대한금속·재료학회
KOREAN INSTITUTE OF METALS AND MATERIALS

4. KIM–JIM Symposium
Room 302, October 25, 2012

Opening comments | 09:00-09:05

Chairman: S.K. Kwon (POSTECH)

KJ-1 | 09:05-09:25

Environment-Dependent Nanomorphology

Aloysius Soon

Yonsei Univ.

KJ-2 | 09:25-09:45

First-principles Study on Mechanical Properties of Dilute Si in Fe-Si Alloy

Y. Chen

Tohoku Univ.

KJ-3 | 09:45-10:05

First-Principles Local-Energy and Local-Stress Calculations of Metallic Grain Boundaries

M. Kohyama

AIST

KJ-4 | 10:05-10:25

All-Electron Mixed Basis Approach as An Accurate First-Principles Method

K. Ohno

Yokohama National Univ.

Coffee Break | 10:25-10:45

Chairman: Y. Chen (Tohoku Univ.)

KJ-5 | 10:45-11:05

Ab initio and Multi-scale Computational Design of High Functional Materials for Renewable Energy Devices

B.C. Han

DGIST

KJ-6 | 11:05-11:25

Effect of a Nickel Cluster on the Dissociation Process of Hydrogen Molecule

R. Sahara

Tohoku Univ.

KJ-7 | 11:25-11:45

Exploring Structures and Phase Relationships of Ceramics at Finite Temperature from First Principles

I. Tanaka

Kyoto Univ.

KJ-8 | 11:45-12:05

Structures of the Generalized Planar Fault Energy in FCC Metals

S.K. Kwon

POSTECH

Lunch | 12:05-13:30

Chairman: P.-R. Cha (Kookmin Univ.)

KJ-9 | 13:30-13:50

Cluster Variation Method and its Applications

T. Mohri

Hokkaido Univ.

KJ-10 | 13:50-14:10

Multi-scale Simulation of Interfacial Roughness Effects in Silicon Nanowires

K.R. Lee

KIST

KJ-11 | 14:10-14:30

Hydrostatic Pressure Dependence of Dislocation Emission Phenomena from Aluminum <112> Tilt Grain Boundaries

T. Shimokawa

Kanazawa Univ.

KJ-12 | 14:30-14:50

Pathways of Conformational Transitions in Molecules

I.-H. Lee

KRISS

Coffee Break | 14:50-15:10

Chairman: M. Ohno (Hokkaido Univ.)

KJ-13 | 15:10-15:30

Phase-field Simulation of Initial Stage Solidification in Continuous Casting of Fe-Mn-C Alloys

W.T. Kim

Cheongju Univ.

KJ-14 | 15:30-15:50

Systematic Materials Design Combining Phase-field Modeling of Microstructure Changes and Image-based Calculation of Materials Properties

T. Koyama

Nagoya Inst. of Tech.

KJ-15 | 15:50-16:10

Effect of Micro-elasticity on Phase Transformations: A Phase Field Study

P.-R. Cha

Kookmin Univ.

KJ-16 | 16:10-16:30

A Microstructure-based Analysis of Deformation Behavior of Metals

H.N. Han

Seoul Nat' l Univ.

Coffee Break | 16:30-16:50

Chairman: I.-H. Lee (KRISS)

KJ-17 | 16:50-17:10

Quantitative Phase-field Modeling of Alloy Solidification: Toward a Large-scale and Highly-accurate Simulation of the Solidification Microstructure

M. Ohno

Hokkaido Univ.

KJ-18 | 17:10-17:30

A Numerical Simulation Study on the Inclusion Behaviors during Secondary Refining Process for Steel

Yi, K.-W.

Seoul Nat' l Univ.

KJ-19 | 17:30-17:50

Multiscale Design of Diffusion-stress Coupled Battery Anode

M. Cho

Seoul Nat' l Univ.

Closing Comments | 17:50-17:55

5. 트라이볼로지 심포지엄
Room 601호, 10월 25일

좌장 : 장호 (고려대학교)

601A-1 | 09:30 **강연**

자동차 샤시 시스템의 개발 동향

*김성수, 하동헌, 안희철

(주)만도.

601A-2 | 10:00

Tribological Behavior of Cr-Nb-N, Cr-Mo-N Coatings Prepared by Hybrid PVD Prepared by Hybrid PVD

*오윤석, 양영환[1], 여인웅[2], 박상진[3], 임대순[1]

한국세라믹기술원. [1]고려대학교. [2]현대기아자동차 연구소. [3]현대하이스코 기술연구소.

601A-3 | 10:20

엔진부품 적용을 위한 TiN-Ag 코팅층의 트라이볼로지 특성 연구

*여인웅, 강혁, 홍웅표, 최광훈, 한도석

현대자동차 중앙연구소.

601A-4 | 10:40

알루미늄의 내마모성 향상을 위한 Ni-Al계 금속간화합물의 연소합성 코팅

*이한영, 김근영[1]

계명대학교. [1]계명대학교대학원.

601A-5 | 11:00

LFT가 첨가된 Poly Propylene 기지소재에 슬립 개선재 첨가에 따른 Scratch 특성

*염현식, 방상호, 김성수

만도신소재.

601A-6 | 11:20

Synthesis and Characterization of Tribological Properties of Ternary BCN Coatings

*김두인, 박종극[1], 김광호

부산대학교. [1]한국과학기술연구원.

601A-7 | 11:40

Effect of Pad Surface Roughness on Material Removal Rate in Chemical Mechanical Polishing Using Ultra Fine Colloidal Ceria Slurry

Sol Han, Hong Jin Kim, Myung Ki Hon, Byoung Ho Kwon, Kuntack Lee, Yongsun Ko

Samsung Electronics.

좌장 : 김성진 (현대자동차)

601B-1 | 13:10

글로벌 공용화를 위한 Fusion 브레이크 마찰재 개발

*한재민, 김성진, 박현달, 권성욱[1]

현대자동차 연구개발본부 첨단재료연구팀. [1]상신브레이크.

601B-2 | 13:30

자동차용 마찰재의 스틱-슬립 발생에 대한 습기의 효과

*이완규, 김성환, 장호

고려대학교 신소재공학과.

601B-3 | 13:50

습도 변화에 따른 Non Steel과 Low Steel 마찰재의 물성 및 시험평가에 관한 연구

*황성은, 김신욱, 편흥식, 이성주, 박병규

KB오토시스(주).

601B-4 | 14:10

자동차용 브레이크 마찰재에서 구리 함량에 따른 마찰 및 마모 특성에 관한 연구

*성상훈, 이정주, 김성진[1], 박현달[1], 장호[2]

상신브레이크(주). [1]현대자동차. [2]고려대학교.

601B-5 | 14:30

자동차 브레이크 PEDAL FEEL 향상을 위한 응답성 개선

*박수열, 박홍규

새론오토모티브.

601B-6 | 14:50

자동차용 브레이크 마찰재의 표면 형상에 따른 접촉강성과 마찰특성

*신민욱, 이상목, 장호

고려대학교.

601B-7 | 15:10

ABS(Antilock Brake System)용 솔레노이드 밸브의 DLC코팅 마찰마모 특성

*하동헌, 김성수, 권태환

(주)만도.

4. KIM-JIM Symposium
Room 302호, 10월 25일

[KJ-1 | 09:05]
Environment-dependent Nanomorphology: Aloysius Soon*; Department of Materials Science and Engineering, Yonsei University, Seoul, Korea
Keywords: computational nanomorphology, density-functional theory, nanothermodynamics

One of the main objectives of nanomaterials modeling is to understand the correlation between an external (or environmental) factor and a desirable chemo-physical property that may be harnessed for some technological gain [1]. In many instances, detailed knowledge of the atomic structure and morphology of the nanoparticle allows us to focus on its structure–property, as well as structure–environment relationships. The atomic structure of the nanoparticle is generally thought to be a function of its local environment, and its chemo-physical properties are then deduced to be a function of its atomic structure. Thus, understanding the structure-environment relationship will enable us to make some informed predictions regarding its structure-property relationship. Consequently, this will bring us one step closer to realizing the dream of designing and tailoring nanoparticles for specific technological applications (e.g. nanocatalysis). In this talk, using a few material systems as examples [2], I will illustrate how the immediate gaseous/aqueous environment could modify the morphology of a metal crystallite, yielding very different nanomorphologies as a function of its atomic chemical potentials. Based on first-principles density-functional theory, the energetics of various low-indexed surfaces (with and without adsorbed gases/solvents) is considered and their stability is determined within the framework of *ab initio* atomistic thermodynamics. Coupling with the Gibbs-Wulff theorem, this allows the determination of the equilibrium crystal shape (i.e. its morphology) as a function of its gaseous/aqueous environment, displaying an atomistic control of nanoparticle shape by manipulating its local gas/solvent environment.

[1] D. Peer, J. M. Karp, S. Hong, O. C. Farokhzad, R. Margalit and R. Langer, *Nature Nanotechnol.* 3, 469 (2007).
[2] X. Duan, O. Warschkow, A. Soon, B. Delley, and C. Stampfl, *Phys. Rev. B* 81, 075430 (2010); T.-H. Lee, B. Delley, C. Stampfl, and A. Soon, *Nanoscale* 4, 5183 (2012).

[KJ-2 | 09:25]
First-principles Study on Mechanical Properties of Dilute Si in Fe-Si Alloy: Ying Chen[1,*], Arkapol Saengdeejing[1], Ken Suzuki[1], Hideo Miura[1], and Tetsuo Mohri[2]; [1]Department of Nanomechanics, School of Engineering, Tohoku University, Sendai, Japan
[2]Division of Materials Science and Engineering, Graduate School of Engineering Hokkaido University, Sapporo, Japan
Keywords: first-principles, mechanical property, Fe-Si

Fe-Si binary alloy has a variety of applications in transformers, motors, and structural materials due to its excellent magnetic and mechanical properties. Some interesting properties have been reported in the bcc-Fe with dilute Si, such as, increasing the Si content from 2-3 to 5-6 wt% improves yield stress whereas the ductility drops sharply at Si 6.5 wt%. In order to understand the mechanism of such change in the mechanical properties with Si concentration, first-principles calculations are performed to Si-doped bcc-Fe up to 6.5 wt.%Si concentration. Using stress-strain method, bulk modulus, shear modulus, and elastic constants have been evaluated for several Si contents based on electronic structures. These calculated mechanical properties vary non-monotonically with the Si concentration, and all show a obvious decrease at around 5.6 wt.%Si. The bulk to shear modulus ratio indicate a ductile to brittle transition based on an empirical rule as the Si content increasing beyond 5.6 wt.%Si. Electronic structures and force constants results revealed the essential difference in Fe-Si bonding characteristic when Si concentration is crossing 5.6wt%Si. The influence of the magnetic property on the mechanical property which is recognized as one of particular features of Fe-Si alloy is further discussed.

[KJ-3 | 09:45]
First-Principles Local-Energy and Local-Stress Calculations of Metallic Grain Boundaries: Masanori Kohyama[1,*], Shingo Tanaka[1], Hao Wang[1], Somesh Bhattacharya[1] and Yoshinori Shiihar[2]; [1]AIST, Japan, [2]University of Tokyo, Japan
Keywords: local density, stress density, PAW method, grain boundary

In the plane-wave DFT schemes, physical quantities such as energy and stress are given as the integral or average throughout the supercell. If such quantities are given in each local region in the supercell, defective systems such as grain boundaries could be deeply analyzed. Historically, local energy-density [1] and stress-density [2] schemes were proposed within plane-wave pseudopotential methods. However, practical applications of such local-energy and local-stress calculations have not been performed enough, due to the difficulty in the gauge-dependent problem. Recently, we have clarified the formulation of the energy and stress densities in the PAW method for the first time [3], and proposed that local energy and local stress can be given as unique physical quantities if the densities are integrated within proper local regions where the gauge-dependent terms are integrated to be zero. This strategy has been successfully applied to each atomic layer of Al (111) surfaces [3] using our package software QMAS (Quantum Materials Simulator) [4]. In this paper, we present our recent applications to grain boundaries in metals such as Al, Cu and Fe. For general

defective systems, it is necessary to define local regions to satisfy the condition for the gauge-dependent problem. We adopt atom-centered regions via fuzzy-Voronoi [5] or Bader integration [6] schemes for such local regions. *Ab initio* results of local energy and local stress are compared with corresponding quantities by EAM potentials. Results indicate that local energy and local stress are very powerful tools to understand the nature of metallic grain boundaries and defects. Acknowledgement: The present study was supported by the Grant-in-Aid for Scientific Research on Innovative Area, "Bulk Nanostructured Metals", by JST Industry-Academia Collaborative Programs, and by the Strategic Programs for Innovative Research, MEXT, and the Computational Materials Science Initiative, Japan.

References:

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[4] S. Ishibashi, T. Tamura, S. Tanaka, M. Kohyama and K. Terakura, http://qmas.jp.
[5] A.D. Beche, J. Chem. Phys. **88**, 2547 (1988).
[6] G. Henkelman, A. Arnaldsson and H. Jonsson, Comp. Mater. Sci. **36**, 354 (2006).

[KJ-4 | 10:05]

All-Electron Mixed Basis Approach as An Accurate First-Principles Method: Kaoru Ohno*,[1], Riichi Kuwahara[1,2], Yoshifumi Noguchi[3], Ryoji Sahara[4], and Yoshiyuki Kawazoe[5]; [1]Department of Physics, Yokohama National University, Yokohama 240-8501, Japan, [2]Accelrys K. K., Kasumigaseki Tokyu Building 17F, 3-7-1 Kasumigaseki, Tokyo 100-0013, Japan, [3]Institute for Solid State Physics, University of Tokyo, Chiba 277-8581, Japan, [4]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, [5]New Industry Creation Hatchery Center, Tohoku University, Sendai 980-8579, Japan

Keywords: first-principles calculation, density functional theory, mixed-basis approach, local density approximation, GW approximation

We have developed the all-electron mixed basis approach (the name of our code is 'TOMBO') in which one-electron wave functions are expanded in a linear combination of both plane waves (PWs) and numerical atomic orbitals (AOs) confined inside non-overlapping atomic spheres. The AOs are described as a product of the radial numerical AO function in logarithmic mesh and the cubic harmonics. The radial AO functions (in particular the valence AOs) are truncated by subtracting a smooth parabolic function that satisfies the matching condition at the radius of the non-overlapping atomic spheres. The method is completely free from the basis set superposition error (BSSE) and mostly prevents the overcompleteness problem. Because we need not to evaluate overlap integrals between neighboring AOs, the related numerical error does not appear. On the other hand, overlap integrals between PW and AO are evaluated by one-dimensional numerical integrations of a product of the spherical Bessel function and the radial AO function in radial logarithmic mesh. The electrostatic and the exchange-correlation potentials within the local density approximation (LDA) of the density functional theory (DFT) are provided in the global (mesh * mesh * mesh) space defined inside the unit cell and also in the non-overlapping atomic spheres. These treatments guarantee the accuracy of the computation. The method can well describe both deeply localized core orbitals and widely extended free-electron-like orbitals with relatively small number of basis functions, and is applicable to variety of systems including atoms, molecules, clusters, surfaces, interfaces, and crystals. TOMBO is now applicable to (1) molecular dynamics within the DFT (or the time-dependent DFT), (2) quasiparticle calculations within the Hartree–Fock approximation (HFA) or more sophisticated approximations based on the many-body perturbation theory, e.g., the GW approximation (GWA) or the second-order (Møller–Plesset) approximation, and (3) optical absorption spectra (or Auger spectra for the two electron emission process) based on the Bethe-Salpeter equation (BSE) beginning with the GW approximation. The program is fully parallelized by using open MP and MPI. We will demonstrate several examples of these calculations. Our present aim is to make up the latest version of our code more user friendly and to open it to the public.

[KJ-5 | 10:45]

Ab initio and Multi-scale Computational Design of High Functional Materials for Renewable Energy Devices: Byungchan Han*, Min Ho Seo, Junkyo Seo, and Seunghyo Noh, Inhye Kwon; Daegu Gyeongbuk Institute of Science & Technology (DGIST), Daegu 711-873, Korea

Keywords: Ab-initio, multi-scale, computation, energy materials, design, high function

A wide commercialization of clean renewable energy systems such as hydrogen fuel cells or Li-ion batteries has been hindered by high cost and low efficiency of the materials. In spite of several decades of concentrated efforts, the progress in the development of high functional energy materials is slow. Largely it is because of the extensive time and financial consuming procedure to discover new materials with an experimental approach. Over the last decade first principles computings have been utilized in a variety of areas, especially in designing of renewable energy materials via its extreme accuracy standing on the quantum mechanics as well as the fast time convergence relying on modern computational architectures that drove such a wide scale of applications. In this talk, it is shown that ab-initio density functional theory (DFT) calculations are very useful for characterizing the electrochemical stability and desired functionality of energy materials. As an example, equilibrium

potential-pH diagrams (Pourbaix diagram) and thermodynamic free energy maps of nano-scale Pt catalysts are calculated, which are of importance in high functional hydrogen fuel cells. Identifying the best alloy elements beyond pure materials are viable through the ab-initio methods combined with aiding from statistical mechanics (cluster expansion theory). It enables multi-scale computations to predict thermodynamic observables of engineering scale materials with ab-initio calculated atomic-scale interactions. This methodology is especially suitable in constructing multi-component phase diagrams and identifying the optimum synthetic path for desired energy materials.

[KJ-6 | 11:05]

Effect of a Nickel Cluster on the Dissociation Process of Hydrogen Molecule: Ryoji Sahara[1,*], Hiroshi Mizuseki[1], Marcel Sluiter[2], Kaoru Ohno[3], and Yoshiyuki Kawazoe[1]; [1]Institute for Materials Research, Tohoku University, Japan, [2]Delft University of Technology, Netherlands, [3]Yokohama National University, Japan

Keywords: hydrogen storage materials, dissociation, first principles

It is said that using the spillover process is efficient to enhance the hydrogen storage capacity of hydrogen storage materials. In the process, hydrogen is transferred from a metal catalyst to hydrogen storage materials. The purpose of the present study is clarification of the dynamics of the spill-over process by explicit consideration of the excited states to improve hydrogen storage capacity to higher densities (6 wt.% or more) in order to facilitate practical use. To the purpose, dissociation process of hydrogen molecule on metal calatyst is studied. A possibility of dissociation of a hydrogen molecule around a nickel dimer is investigated as a simple but important example of the initial stage of the hydrogen spill-over process, which is a candidate to enhance the hydrogen storage capacity. The electron and the ion dynamics are analyzed employing Ehrenfest's theorem and solving the time-dependent Kohn-Sham equation of time-dependentdensity functional theory coupled with the Newtonian equation of motion. We use TOhoku Mixed-Basis Orbitals ab initio program TOMBO developed by our research group, which enables us to study based on "all-electron mixed-basis approach" with smaller number of plane waves [1,2]. The hydrogen molecule starts to dissociate under one electron excitation from the highest occupied molecular orbital level to the lowest unoccupied molecular orbital level, while the exited electron level crosses the lower hole level yielding an energy gain [3]. A part of this work has been supported by New Energy and Industrial Technology Development Organization (NEDO) under "Advanced Fundamental Research Project on Hydrogen Storage Materials". The authors would like to express their sincere thanks to the staff of the Center for Computational Materials Science of the Institute for Materials Research, Tohoku University for their continuous support of the supercomputing facilities.

References

[1] K. Ohno, K. Esfarjani, and Y. Kawazoe, Computational Materials Science: From ab initio to Monte Carlo Methods, Springer Series in Solid-State Sciences Vol. 129 (Springer-Verlag, Berlin, Heidelberg, 1999), 42-46.
[2] M. S. Bahramy, M.H.F. Sluiter, and Y. Kawazoe, Phys. Rev. B 73, 045111 (2006).
[3] R. Sahrara, H. Mizuseki, M. H. F. Sluiter, K. Ohno, and Y. Kawazoe, in preparation.

[KJ-7 | 11:25]

Exploring Structures and Phase Relationships of Ceramics at Finite Temperature from First Principles: Isao Tanaka[1,2,*], Atsushi Togo[1], and Atsuto Seko[1]; [1]Department of Materials Science and Engineering, Kyoto University, Japan, [2]Nanostructures Research Laboratory, Japan Fine Ceramics Center, Japan

Keywords: oxide, ionic conductor, cluster expansion, phonon, phase transition

First principles calculations on the basis of density functional theory (DFT) have been developed over the last few decades. Progress of computational powers and techniques is remarkable during this period. Crystals with several hundreds of atoms can be routinely examined by the DFT methods using personal computers these days. When clustered computers are employed, DFT calculations of periodic units composed of several thousands of atoms can be done without much technical difficulties. Today one can also perform a large set of DFT calculations systematically with high numerical accuracy. Capability of a large set of calculations is often more important in materials science community than a large size calculation, since the information can be used to evaluate thermodynamical quantities. When statistical thermodynamics is combined with a systematic set of first principles calculations, the configurational and vibrational contributions to thermodynamical quantities and their temperature dependence can be evaluated. When phonon states are obtained, the products and pathways of phase transitions can also be analyzed on the basis of the information of imaginary phonon modes. Such theoretical results can not only "reproduce" available experimental data but also "predict" as-yet-unknown structures and properties. Even when experimental data were reported, they are sometimes widely scattered or conflicting. Then theoretical calculations can be used to adjudicate upon the arguments. In this talk I show many examples how we use DFT methods in conjunction with lattice dynamics and statistical thermodynamics simulations to elucidate structures and phase relationships of selected ceramic materials.

[KJ-8 | 11:45]

Structures of the Generalized Planar Fault Energy in FCC Metals: Minho Jo, Y.M. Koo, and S.K Kwon*; Graduate Institute of Ferrous Technology, Pohang

University of Science and Technology, Korea
Keywords: plastic deformation, face-centered cubic metals, stacking fault energy, generalized planar fault energy

It is still a challenging task to build a microscopic theory of plasticity in face-centered cubic metals. While an empirical description of plastic deformation in terms of the stacking fault energy is widely accepted in materials science, its physical basis is weak. It is questionable whether the single energy parameter which lacks energy barrier information could reliably describe the complex pictures of plastic deformation. In contrast, the generalized planar fault energy from advanced atomic theory provides energy barrier information but is not yet fully appreciated because of its inaccessibility from experiments. Here, we try to reconcile the both sides in a unified view by exploring the physical implications of the generalized planar fault energy curve. Some perspectives of structural materials development are also suggested.

[KJ-9 | 13:30]

Cluster Variation Method and its Applications: Tetsuo Mohri*; Research Center for Integrative Mathematics and Division of Materials Science & Engineering, Faculty of Engineering, Hokkaido University, Sapporo 060-8628, Japan
Keywords: cluster variation method, continuous displacement cluster variation method, spinodal ordering temperature, first-principles phase field calculations

Bragg-Williams approximation has been most widely employed in various alloy phase equiibria calculations. This is due to the mathematical simplicity in extending it to various crystal structures and multicomponent alloy systems. It has been, however, pointed out that Bragg-Williams approximation does not provide an accurate result in the calculated topology of the phase boundaries and the order of the transition. The deficiencies of the Bragg-Williams approximation are ascribed to the neglect of configurational correlations. Cluster Variation Method (CVM), on the other hand, has been regarded as one of the most reliable theoretical tools in dealing with atomic correlations which are of central importance in the phase equilibria and phase transitions. By combining CVM with electronic structure total energy calculations, even the first-principles phase equilibria calculations have been attempted. One of the difficulties of the CVM, however, stems from the fact that one needs to deal with multi-valued free energy function, therefore both the formulation and numerical minimization of the free energy are not a simple task. Yet, along with the development of numerical schemes as well as powerful computers, we are at the verge of extending CVM to various intriguing phonemena in alloy systems. In the present talk, the author introduces several new directions of the applications of the CVM. One is the first-principles stability analysis of configurational fluctuation in alloys which has been known as spinodal ordering. The Fourier transformation of the second order derivative matrix of the free energy provides the stability locus in the calculated phase diagram, which can be utilized to analyze the intrinsic stability of the system against configurational fluctuation. The second one is the calculation of local atomic displacement. In order to calculate an accurate phase diagram, it is deemed essential to introduce additional freedom of the atomic displacement in addition to configurational freedom. Recent development of Continuous Displacement Cluster Variation Method is the key to this calculation. The last one is the analysis of the dislocation core structure. By extending the basic cluster in two dimensional directions to build a supercell, one can gain the information of atomistic configuration around the extended defects. We demonstrate the results of superpartial dislocations in an ordered compound.

[KJ-10 | 13:50]

Multi-scale Simulation of Interfacial Roughness Effects in Silicon Nanowires: Byung-Hyun Kim[1,2], Hyo-Eun Jung[3], Mincheol Shin[3] , Yong-Chae Chung[2] and Kwang-Ryeol Lee[1]*; [1]Computational Science Research Center, Korea Institute of Science and Technology, Korea, [2]Division of Materials Science and Engineering, Hanyang University, Korea, [3]Department of Electrical Engineering, Korea Advanced Institute of Science and Technology, Korea
Keywords: Please specify keywords of your abstract (less than five keywords)

Understanding and controlling the interface morphology of Si/SiO2 in silicon nanowires (SiNWs) is an essential issue in optimizing the device performance of SiNW field effect transistors (FETs). However, experimental methods to characterize the interfacial roughness are highly limited at present. Previous analysis on the effect of the interfacial roughness in SiNWs were thus based on pure speculation [1]. In this work, we investigated the effect of the interfacial roughness on the transport behavior by using an atomic scale simulation of SiNW oxidation combined with an interface roughness characterization technique and the non-equilibrium Green's function (NEGF) calculation. The present work reveals that RMS and the correlation length increase with increase of the oxidation time, while they decrease with the diameter of SiNWs due to the residual stress in the interface region between Si/SiO_2. The latter gives the effect of enhancing the SR limited mobility, compared to the case of using the bulk values.

[KJ-11 | 14:10]

Hydrostatic Pressure Dependence of Dislocation Emission Phenomena from Aluminum <112> Tilt Grain Boundaries: Tomotsugu Shimokawa* and Kazuki Horikawa: Kanazawa University, Japan
Keywords: grain boundary, dislocation, atomic simulation, hydrostatic pressure, dislocation source

When the grain size of polycrystalline metals decreases to less than 1ìm (commonly referred to as ultrafine-grained (UFG) metals or nanocrystalline metals), the mechanical properties of UFG metals become different from that of

coarser-grained metals. One of the examples is that UFG metals show tension/compression asymmetry of strength (S. Cheng, Acta Mater. 51, 4505(2003).), that is, hydrostatic pressure dependence of plastic deformation occurs in UFG metals. The obvious difference between coarse-grained and UFG metals is the volume fraction of grain boundaries, which increases dramatically as the grain size decreases to 100 nm. Therefore, grain-boundary-mediated plasticity; a transition of starting points of plastic deformation from insides of each grain to interfaces between grains, could control the unique mechanical properties of UFG metals. However, it has not been easy to research the detailed generation mechanism of plastic deformation from the interfaces by only experimental and theoretical approaches because of the complicated structures of interfaces generally having five degrees of freedom macroscopically and three degrees of freedom microscopically. In this study, we use atomic simulations to investigate the effect of interface structures on the ability of grain boundaries to generate plastic deformation (T. Shimokawa, Phys. Rev. B, 82, 174122(2010).) and also investigate the hydrostatic pressure dependence of dislocation emission phenomena from aluminum <112> tilt grain boundaries. Using the slope of the hydrostatic pressure dependence of the resolved shear stress to the dislocation emission from S21 and S15 boundaries obtained by atomic simulation, we will compare the result obtained from atomic simulation with the experiment of tension–compression asymmetry of strength of UFG aluminum.

[KJ-12 | 14:30]

Pathways of Conformational Transitions in Molecules: In-Ho Lee; Korea Research Institute of Standards and Science (KRISS), Daejeon 305-340, Korea

Keywords: transition path, reaction coordinate, action, molecular dynamics

The trajectories carrying the molecule over the potential-energy barrier are called transition paths. It is the transition-path trajectories where conformational change occurs. Discerning transition-path trajectories holds the essential ingredients for understanding of the chemical reaction, in general. I will present dynamical pathway models of those various structural transformations in molecules and nanostructures, using action-derived molecular dynamics proposed for the simulation of infrequent-event systems. I will explain how this approach can be used in the simulation and modeling of condensed phase and biomolecular systems. The related examples will provide us the insight for understanding the physical and chemical mechanisms of the atomic-level reactions between various molecules and nanostructures. Atomically detailed interactions through a many-body potential are used to compute the fullerene formation, fullerene fusion, catalytic fullerene fusions, metal defect formations in fcc metals, screw-dislocation formations in Cu, vacancy diffusions in carbon nanotubes, and protein folding pathways. Full details of the protocol will be demonstrated and discussed. Numerical results derived from several simulations place emphasis on the computational merits of the protocol. I will utilize to the fullest extent of the reaction coordinates obtained from the protocol and present an additional protocol for characterizing the conformational changes. I will summarize several applications of the method and challenges related to the Markov state model, weighted-ensemble dynamics, replica-exchange molecular dynamics, principal component analysis, and Crooks' fluctuation theorem.

[KJ-13 | 15:10]

Phase-field Simulation of Initial Stage Solidification in Continuous Casting of Fe-Mn-C Alloys: S.G.Kim[1], W.T. Kim[2,*], Y.B.Park[3], P.R.Cha[4], H.Y.Seo[5] and J.T. Choi[5]; [1]Dept. of Materials Science and Engineering, Kunsan National University, Kunsan, Korea, [2]Dept. of Optical Engineering, Cheongju University, Cheongju, Korea, [3]Dept. of Materials Science and Engineering, Sunchon National University, Korea, [4]School of Materials Science and Engineering, Kookmin University, Seoul, Korea, [5]Technical Research Center, Hyundai Steel Company, Dangjin, Korea

The carbon steels of hypoperitectic compositions often develop significant undulations on the solidified shell/mold interface at the initial stage of solidification during continuous casting. The first step to understand the origin of this anomalous solidification behavior is to directly simulate the microstructure evolution during solidification. In this study, we developed a phase-field method to simulate the microstructure evolution during solidification of nonisothermal, multicomponent (Fe-Mn-C) and multiphase system (liquid, ferrite and austenite phases) under real process conditions. To enhance the computational efficiency, we reformulated the original thermodynamic database of Fe-Mn-C alloy into a new database on compositions as functions of chemical potentials. We report the basic characteristics of the simulated microstructures.

[KJ-14 | 15:30]

Systematic Materials Design Combining Phase-field Modeling of Microstructure Changes and Image-based Calculation of Materials Properties: Toshiyuki Koyama*; Nagoya Institute of Technology, Japan

Keywords: phase-field method, phase transformations, stress-strain curve, magnetic hysteresis, dielectric hysteresis

Phase-field method has recently been extended and utilized across many fields in materials science for analyzing and modeling the heterogeneous microstructure changes [1-4]. Since this method can systematically incorporate the effect of coherent strain induced by lattice mismatch and applied stress as well as the external electric and magnetic fields, it has been applied to many material processes including solidification, solid-state phase transformations and various types of complex microstructure changes. In this study, firstly the calculation method of phase-field approach is briefly

explained. In particular, the basic philosophy of phase-field simulation is mentioned [3]. Secondly, we summarize the recent calculation results of the phase-field simulation of phase transformations in various materials [1]. Finally, the image-based calculations of materials properties are explained, where the simulated microstructure image that is the output data of phase-field simulation is employed as a boundary condition for calculating the materials properties. We demonstrate the cases of the mechanical property (stress-strain curve) [2], magnetic property (magnetic hysteresis) [1] and electric property (dielectric hysteresis) [3] as typical examples of this approach.

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[KJ-15 | 15:50]

Effect of Micro-elasticity on Phase Transformations: A Phase Field Study: Pil-Ryung Cha[1,*], Dong-Uk Kim[1], Won Tae Kim[2], and Seong Gyoon Kim[3]; [1]School of Advanced Materials Engineering, Kookmin University, Seoul 135-702, Korea, [2]Department of Optical Engineering, Cheongju University, Cheongju 360-764, Korea, [3]Department of Materials Science and Engineering, Kunsan University, Kunsan 573-701, Korea

Keywords: micro-elasticity, phase field model, particle splitting, g-a transformation, grain growth, texture

Both the internal stress occurring during phase transformation and the external stress caused by an external constraint affect remarkably the thermodynamics, kinetics and microstructural evolution of phase transformation. These effects of micro-elasticity on various phase formations have been studied for a long time and much progress has been achieved. Particularly, recent development of the phase field model with micro-elasticity opened a new avenue for the investigation of the micro-elasticity effect in real microstructures. In this presentation, the phase field model considering both the internal and external stress fields is presented and the effect of micro-elasticity on various phase transformation phenomena is discussed using the model. The phase transformation phenomena considered in this presentation are as follows: particle splitting in Ni-based superalloys, γ-α transformation in Fe-Mn-C alloy, and grain growth and texture evolution in Cu, Fe and Mg.

[KJ-16 | 16:10]

A Microstructure-based Analysis of Deformation Behavior of Metals: Heung Nam Han; Department of Materials Science and Engineering and Center for Iron & Steel Research, RIAM, Seoul National University, Seoul 151-744, Republic of Korea

In first part of the presentation, the microstructural changes in individual ferrite grains in single (so called interstitial-free or IF) and dual phase (DP) steel sheets under a series of equi-biaxial tensile deformations will be discussed, which were observed by orientation imaging microscopy (OIM) with a special equi-biaxial tensile device. The individual deformed microstructures were compared with the corresponding results from viscoplastic simulations using the Fast Fourier transform (FFT) method. For a quantitative analysis of the effect of the hard martensite phase on the microstructural changes and variation of the surface height in the ferrite regions of the DP steel under equi-biaxial tensile deformation, additional simulations, where the martensite grains were replaced with ferrite grains (monolithic case), were performed and the results were also compared with those from the simulations on the DP steel (DP case). It was found that the main effect of the hard martensite islands on the viscoplastic response in the DP steel under equi-biaxial tensile deformation was that the strain was highly concentrated on the adjacent ferrite grains and a corresponding significant variation in surface height was induced, which resulted in strain gradients, orientation dispersion and geometrically necessary dislocations (GNDs) in the ferrite grains. In second part, a dislocation density based constitutive equations of polycrystalline materials were implemented into to a full-field formulation based on fast Fourier transforms (FFTs) for the analysis of viscoplastic local response. The slip resistance of each slip system was computed based on densities of both statistically necessary dislocations (SSDs) and geometrically necessary dislocations (GNDs). It was shown that the suggested model could describe a grain-size dependant mechanical response corresponding to the Hall-Petch effect. In addition, the grain size effects on microstrutural change such as the subgrain texture evolution, the intra- or inter- granular misorientation distribution and the orientation gradient in grains during deformation will be discussed.

[KJ17 | 16:50]

Quantitative Phase-field Modeling of Alloy Solidification: Toward a Large-scale and Highly-accurate Simulation of the Solidification Microstructure: Munekazu Ohno*; Faculty of Engineering, Hokkaido University, Japan

Keywords: phase-field model, solidification, microstructure, dendrite

The phase-field model is a powerful tool to describe microstructural pattern formation during alloy solidification. Although its capability of affording qualitative understanding of phenomena is generally acknowledged, a longstanding issue remains unresolved regarding the quantitative aspect. Early models have been developed so as to reproduce the free-boundary problem of interest in the so-called sharp-interface limit where the thickness of the diffuse interface *W*

is approximated to zero. However, it is prerequisite for this diffuse interface approach to employ a finite value of W in practice. A typical value of W for the solid-liquid interface is a few nm, thus it needs a mesh size of Å-order to describe the diffuse interface. This limits the system size to extremely small, making it impossible to deal with problems on the microstructural scale. Therefore, W has to be increased by orders of magnitude from the realistic thickness. This increment, in turn, unrealistically magnifies some physical effects, the contributions of which scale with W, and it accordingly precludes quantitatively correct simulations. A way out of this impasse was proposed by Karma and Rappel. They put forward a model based on a new procedure called the thin-interface limit in which W is taken to be smaller than any physical length appearing on the microstructural scale but is much larger than the realistic thickness. This model is called the quantitative phase-field model in that it enables quantitatively meaningful simulations. However, the quantitative modeling has so far been developed only for some specific systems. An important step toward further generalization is to model alloy solidification involving coupled heat and solute diffusion in multicomponent alloys. This is tackled in this study. In this study, the model was developed based on the thin-interface asymptotics on time evolution equations of the phase-field model. The solutal and thermal antitrapping current terms were formulated to describe non-isothermal solidification in multi-component alloys with arbitrary diffusivities. The performance of the model was investigated by conducting the convergence test of the simulation outcome with respect to W. We focused on free dendritic growth into undercooled melt in ternary alloys. Reasonable convergence was demonstrated regarding dendrite tip velocity, radius and concentration profiles in the steady state growth. Hence, quantitatively accurate outcome can be obtained for finite values of W in this model. This fact opens the way for a large-scale computation of the solidification microstructure, since the computational cost of the phase-field simulations is proportional to W^{-5}. The present model can be utilized to describe and predict the solidification microstructure in practical alloys with high accuracy.

[KJ-18 | 17:10]

A Numerical Simulation Study on the Inclusion Behaviors during Secondary Refining Process for Steel: Yi Kyung-woo*; Seoul National University, Seoul, Korea

Keywords: inclusion, secondary refining, integrated model, steelmaking

Because large amount of oxygen remains after converter refining process of steel, the oxygen should be removed after the process. To remove oxygen from refined steel melt, metals with stronger oxygen affinity, such as aluminum, silicon, calcium or magnesium, are put into the melt during the additional refining process, usually called secondary refining process. The metals form stable oxides in the melt. If the amount of metal is sufficient to react with oxygen in the melt, nearly all the oxygen of the melt formed oxides with the metals and oxygen contents of melt becomes very low (as an example a few ppm for aluminum). But, the reacted oxides remain in the steel metal. Because the density of the inclusions is usually very smaller than the melt, the inclusions should rise up to the melt surface. So, all the inclusions incorporated in the slag on top of the melt after some time. However, small oxides tend to follow fluid flow of melt and remains long time in the melt. These remained oxides become non-metallic inclusions after casting and cause many problems when the casted steel is used as cold rolled sheet. The present study suggest an integrated model for predict the inclusion behavior during secondary refining process. Modeling of inclusion dynamics, thermodynamics, fluid flow and multi-phase behavior should be incorporated in the model. The developed model quantitatively predicts the change of contents and special distributions of the oxides. Experimental data obtained during field operations are compared to verify the model.

[KJ-19 | 17:30]

Multiscale Design of Diffusion-stress Coupled Battery Anode: Maenghyo Cho[1]*, Kyeongjae Cho[1,2], Seongmin Chang[1], and Janghyuk Moon[1]; [1]WCU Multiscale Mechanical Design, School of Mech and Aero Eng, Seoul National University, Seoul, Korea, [2]Department of Material Science and Engineering, University of Texas, Dallas, USA

Keywords: multiscale, li-ion battery, DFT, diffusion, continuum

Multiscale simulation for Li-ion battery anode is performed. Elastic stiffnesses and diffusion coefficients of various combination of Li and Si alloy are obtained from DFT simulations. Diffusion-stress coupled multiphysics simulations are carried out in continuum level via finite element method. Stiffness values of Li_x Si and diffusion constant values of Li, and Si compound obtained from DFT simulation are mapped to each element of FEA(Finite Element Analysis). This process is, so called, sequential multiscale process. Based on this multiscale analysis, we propose the guideline of design of battery electrode with the design parameters such as shape, size, and hollowness. The critical design envelope for various charge rate, radius of Si wire, and aspect ratio is provided.

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