CALPHAD XXXIX

An International Conference on

Phase Diagram Calculations

and

Computational Thermochemistry

Provisional Program

May 23-28, 2010

Ramada Plaza Jeju

Jeju, Korea

Organizing Committee

Byeong-Joo Lee, Pohang University of Science and Technology (POSTECH)
Chang-Seok Oh, Korea Institute of Materials Science (KIMS)
Joonho Lee, Korea University
Jae-Hyeok Shim, Korea Institute of Science and Technology (KIST)
Hyuck Mo Lee, Korea Advanced Institute of Science and Technology (KAIST)

Co-organized by The Korea Institute of Metals and Materials
Metals Bank, Korea Institute of Materials Science

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Program at a Glance

Venue

Ramada Plaza Jeju Hotel

1255 Samdo2-dong, Jeju City, Jeju 690-032, Korea

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http://www.ramadajeju.co.kr

Transportation

The most convenient public transportation to and from the Jeju International Airport is a taxi service. You may take a taxi at short-distance taxi stand at the front of passenger terminal.

Distance about 4km / taxi fare approx. 3,500 KRW / about 10min.'s ride

General Information

Poster Presentation

The poster will be on display from Monday morning to Wednesday morning in the Halla Hall (8F). Poster size should be less than 90 × 130 cm in either portrait or landscape format. Poster boards and Velcro will be provided. Posters should be mounted on the poster boards no later than 18:00 on Monday and authors are recommended to remove his/her poster before Wednesday noon.

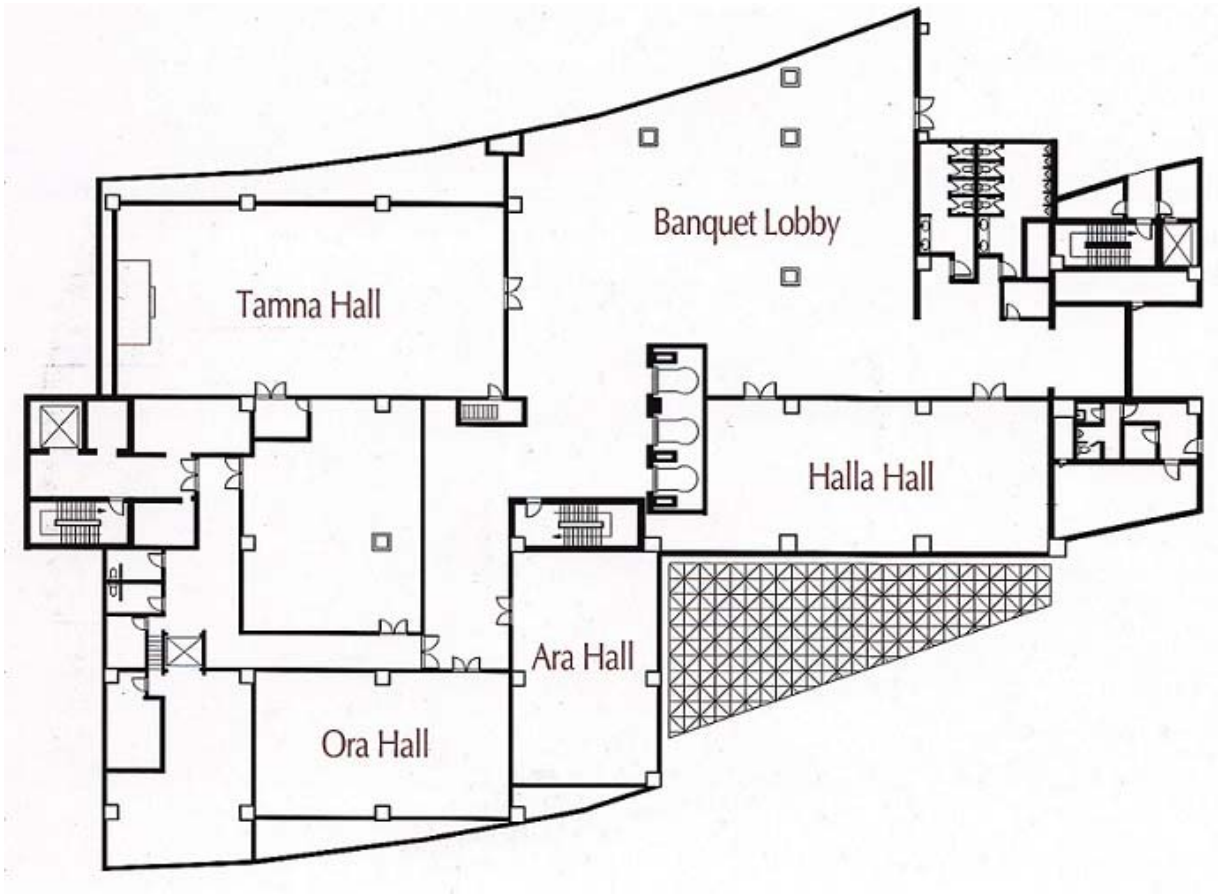
Electricity

The standard voltage is 220 volts and the outlet has two round holes used in many countries.

Internet Service

The internet service will be available in secretary room (Ora Hall) as well as guest rooms.

Map of Session Room



8F
Ramada Plaza Jeju Hotel

- **Session room** **Tamna Hall**
- **Posters** **Halla Hall**
- **Internet connections** **Ora Hall**
- **Secretary** **Ora Hall**

Official and Social Programs

Registration (May 23, 2010)

14:00 to 18:00	Entrance Hall (1F)
After 18:00 (Sun)	Lobby (8F)

Welcome Reception (May 23, 2010)

18:30 to 21:00	Banquet Lobby (8F)

Conference Dinner (May 26, 2010)

18:30 to 21:30	Tamna Hall (8F)

General Meal Times

Breakfast	07:00 to 08:00 at Banquet Lobby (8F)
Lunch	12:30 to 13:30 at Banquet Lobby (8F) * 12:10 to 13:00 (Wednesday)
Dinner	18:30 to 20:00 at Banquet Lobby (8F)
Coffee Break	10:10 to 10:40 at Lobby (8F) 15:30 to 16:00 at Lobby (8F)

Conference Excursion

Wed	13:00 to 17:30	Jeju Forkvillage (at Pyoseon Area)

Accompanying Person Program

Mon	10:30 to 17:00	Seongsan Sunrise Park and Boat Trip to Udo
Tue	10:00 to 16:00	Jeju Botanical Garden and Sulloc Green Tea Museum
Thu	10:00 to 16:00	Seogwipo Area

Session Program

Day 1 : Monday, May 24

- Session 1 : First principles calculations and cluster variation method
- Session 2 : First principles and atomistic calculations
- Session 3 : CALPHAD approach related to alloy systems – I
- Session 4 : CALPHAD approach related to alloy systems – II

Day 2 : Tuseday, May 25

- Session 5 : Modeling of thermodynamic properties and liquid solutions
- Session 6 : CALPHAD approach related to alloy systems – III
- Session 7 : CALPHAD assessment of non-metallic systems – I
- Session 8 : CALPHAD assessment of non-metallic systems – II

Day 3 : Wednesday, May 26

- Session 9 : Lattice stability / Experiments that need thermodynamic analysis – I
- Session 10 : Experiments that need thermodynamic analysis – II

Day 4 : Thursday, May 27

- Session 11 : CALPHAD approach related to ferrous alloys – I
- Session 12 : CALPHAD approach related to ferrous alloys – II
- Session 13 : Database/Software and CALPHAD assessment of metal-hydrogen system
- Session 14 : CALPHAD approach related to thin films and phase field methods

Day 5 : Friday, May 28

- Session 15 : Phase stability of alloy systems – I
- Session 16 : Phase stability of alloy systems – II

Monday (Morning), May 24

08:20	Opening and welcome address (Hyuck Mo Lee and Byeong-Joo Lee)
Session 1 : First principles calculations and cluster variation method Chair : Marcel H.F. Sluiter / George Kaptay	
[O1] 08:30	*Tetsuo Mohri* Challenges in the theoretical calculations of phase equilibria and phase transforma-tion by CVM
[O2] 08:50	*Pablo G. Gonzales-Ormeño, Luiz T. F. Eleno and Cláudio G. Schön* Alloying iron aluminides: fundamental investigation of the metastable b.c.c. phase equilibria in systems Fe-Al-M (M = Mo, Nb, Ti)
[O3] 09:10	*Erwin Hueger, Tomas Kana and Mojmir Sob* *Ab-initio* study of blocking of hcp-fcc phase transformation in Pd thin films by domain boundaries
[O4] 09:30	*J. Pavlů, J. Vřešťál, X.-Q. Chen and P. Rogl* Stability of Laves phases in the Ta-V system
[O5] 19:50	*Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer* *Ab-initio* concepts for an efficient and accurate determination of thermodynamic properties up to the melting point
10:10	Coffee Break (30min)
Session 2 : First principles and atomistic calculations Chair : Tetsuo Mohri / Mojmir Sob	
[O6] 10:40	*Marcel H.F. Sluiter and Emre S. Tasci* Liquid structure as a guide for phase stability in the solid state: prediction of stable compounds in the Au-Si and Au-Ge alloy systems
[O7] 11:00	*Yi Kong and Yong Du* Phase stability of Pr-Pt binary system
[O8] 11:20	*F. Körmann, A. Dick, T. Hickel and J. Neugebauer* First principles concepts to determine the heat capacity of Fe-based alloys
[O9] 11:40	*George Kaptay* Equilibrium in nano-materials with special emphasis to the Al-Ti-C system
[O10] 12:00	*Byeong-Joo Lee* Recent progress in atomistic simulations for nano or nano-structured materials
12:30	Lunch

Monday (Afternoon), May 24

Session 3 : CALPHAD approach related to alloy systems - I Chair : Rainer Schmid-Fetzer / Yong Du	
[O11] 14:00	*Zi-Kui Liu* Building the infrastructure for materials design based on computational thermodynamics
[O12] 14:20	*Libin Liu, Ligang Zhang, Haiying Qi, Guoxing Huang and Yong Du* Thermodynamic database for Mg based alloy systems
[O13] 14:40	*Liling Jin, Youn-Bae Kang and Patrice Chartrand* Modeling of thermodynamic properties and phase equilibria in Mg-Al-Mischmetal systems
[O14] 15:00	*Yinan Zhang, Dmytro Kevorkov, Mamoun Medraj, Jian Li and Elhachmi Essadiqi* Experimental investigation of the Mg-Zn-Ca system via diffusion couples and key experiments
[O15] 15:20	*M. Medraj, M.N. Khan, M. Aljarrah and J.T. Wood* Investigation of the solidification behavior of commercial Mg alloys through experiments and thermodynamic calculations
15:40	Coffee Break (30min)
Session 4 : CALPHAD approach related to alloy systems - II Chair : Zi-Kiu Liu / Liblin Liu	
[O16] 16:10	*Artem Kozlov, Joachim Gröbner and Rainer Schmid-Fetzer* What can we learn about the Mg-Si-Sn-(Ca) system from solidification of aluminum alloy W319?
[O17] 16:30	*Pavel Broz and Jiri Bursik* Theoretical and experimental study of phase equilibria in the Al-Ni-Zn system
[O18] 16:50	*Erwin Povoden-Karadeniz, Piotr Warczok, P. Lang, A. Falahati and E. Kozeschnik* A thermodynamic model of Güinier-Preston-zones in the Al-Mg-Si system
[O19] 17:10	*Jean-Claude Crivello, Mauro Palumbo, Taichi Abe and Jean-Marc Joubert* First *ab initio* calculation of a σ-phase in a ternary system: Cr-Mo-Re
[O20] 17:30	*Yong Du, Lijun Zhang, Dandan Liu, Senlin Cui, Weibin Zhang, Dongdong Zhao, Honghui Xu and Shuhong Liu* Atomic mobility and diffusivity for fcc phase in Al alloys
18:30	Dinner
20:00	Poster Session

Tuesday (Morning), May 25

Session 5 : Modeling of thermodynamic properties and liquid solutions Chair : Jean-Claude Tédnac / Nathalie Dupin	
[O21] 08:30	*Bo Sundman, Malin Selleby and Mats Hillert* An attempt to correct the quasi-chemical model for liquids
[O22] 08:50	*Youn-Bae Kang and Arthur D. Pelton* Modeling short-range ordering and clustering in liquid solutions
[O23] 09:10	*In-Ho Jung and Pierre Hudon* Thermodynamic modeling of phosphate glass system
[O24] 09:30	*Liya A. Dreval', Mikhail A. Turchanin, Alexander R. Abdulov and Pavel G. Agraval* Mixing enthalpies of liquid alloys and thermodynamic assessments of the Cu–Fe–TM (TM = V, Cr, Co, Ni) systems
[O25] 09:50	*Xiao-Gang Lu* Modeling of thermodynamic and thermophysical properties
10:10	Coffee Break (30min)
Session 6 : CALPHAD approach related to alloy systems - III Chair : Bo Sundman / Xiao-Gang Lu	
[O26] 10:40	*Jean-Claude Tedenac and Catherine Colinet* Phase stability of titanium rich intermetallic phases in the Ti-X (X: Al, Ga, Si, Sn) systems
[O27] 11:00	*Johan Bratberg, Bo Sundman and Nathalie Dupin* Application of the combined CEF to the description of the σ phase in the Pd-Ta system
[O28] 11:20	*DongEung Kim, Venkateswara Rao Manga, Shun-Li Shang and Zi-Kui Liu* Thermodynamic modeling of Al-Ni-Pt system using a 4-sublattice model
[O29] 11:40	*V.M. Chad, F. Ferreira, P.B. Fernandes, G.C. Coelho and C.A. Nunes* Thermodynamic Modeling of the Ta–B System
[O30] 12:00	*Nathalie Dupin, Christine Guéneau, Chantal Martial, Jean-Christophe Dumas, Christian Chatillon and Bo Sundman* Reassessment of the thermodynamic description of the (U-Pu-C) system
12:30	Lunch

Tuesday (Afternoon), May 25

Session 7 : CALPHAD assessment of non-metallic systems - I Chair : Patrice Chartrand / In-Ho Jung	
[O31] 14:00	*Bruno N. Stoco and André Costa e Silva* Estimating viscosities in steelmaking slags with basis on a thermodynamic model-Applications in the CaO-Al_2O_3-MgO-SiO_2 system
[O32] 14:20	*Hans J. Seifert, Zhu Pan, Olga Fabrichnaya, Roland Neher, Kristina Brandt and Mathias Herrmann* Thermodynamic evaluation of the Si-C-Al-Y-O system and applications for liquid phase sintering of silicon carbide ceramics
[O33] 14:40	*Sulata Kumari Sahu, C.V. Vishnu Vardhan, Rajesh Ganesan and T. Gnanasekaran* Phase diagram and thermo-chemical studies on Pb-Fe-O system
[O34] 15:00	*Ming Chen, Christodoulos Chatzichristodoulou, Jacob R. Bowen, and Yi-Lin Liu* Experimental investigations and re-modeling of the $LaO_{1.5}$-MnO_x-ZrO_2 system
[O35] 15:20	*Jeroen Heulens, Nele Moelans, Bart Blanpain and Patrick Wollants* Phase field modeling of isothermal crystallization of metallurgical slags using FACT thermodynamic databases for oxide systems
15:40	Coffee Break (30min)
Session 8 : CALPHAD assessment of non-metallic systems - II Chair : André Costa e Silva / Hans J. Seifert	
[O36] 16:10	*Sergei A. Decterov, A. Nicholas Grundy, Eli Brosh, Wan-Yi Kim, Eve Belisle, Christopher Bale and Arthur D. Pelton* Linking thermodynamics, structure and viscosity of oxide melts
[O37] 16:30	*Wan-Yi Kim, Arthur D. Pelton and Sergei A. Decterov* Extended viscosity model for the glass region of oxides solutions
[O38] 16:50	*Guillaume Lambotte and Patrice Chartrand* Assessment of the quaternary reciprocal system Al, Na, Si // F, O: a thermodynamic approach to the corrosion of the refractory lining in aluminum electrolysis cell
[O39] 17:10	*Elizabeth Renaud, Christian Robelin and Patrice Chartrand* Thermodynamic evaluation and optimization of the Na^+, Ca^{2+}, Al^{3+}, Fe^{2+}, Fe^{3+} // F^-, O^{2-}, Va^- system
[O40] 17:30	*Pertti Koukkari, Risto Pajarre and Klaus Hack* Ten years of using advanced Gibbs'ian methods through spreadsheets
18:30	Dinner
20:00	Poster Presentation

Wednesday (Morning), May 26

Session 9 : Lattice stability / experiments that need thermodynamic analysis - I Chair : John Ågren / Hyuck Mo Lee	
[O41] 08:30	*Larry Kaufman* Third generation of lattice stabilities for metals
[O42] 08:50	*Mauro Palumbo, Malin Selleby, Bo Sundman, Tilman Hickel and Suzana G. Fries* On the lattice stabilities of pure Cr and pure Fe
[I-1] 09:10	*Nack J. Kim* Microstructure and texture evolution of twin-roll cast magnesium alloys during thermo-mechanical treatments
[I-2] 09:40	*Nong-Moon Hwang* Diamond deposition with simultaneous graphite etching: Thermodynamic paradox or indication of diamond deposition by gas phase nuclei?
10:10	Coffee Break (20min)
Session 10 : Experiments that need thermodynamic analysis - II Chair : Chang-Seok Oh / Jae-Hyeok Shim	
[I-3] 10:30	*Young Whan Cho* Review on available thermodynamic database of complex metal hydrides
[I-4] 11:00	*Moon-Ho Jo* Vectorial growth of VLS semiconductor nanowires: Thermodynamics vs. kinetics
[I-5] 11:30	*Sang Ho Oh* Atomic-scale observations of phase transformations in nano-sized materials: Deviations from the bulk behaviors
12:10	Lunch

13:00 ~ 17:30	Conference excursion
18:30 ~ 21:30	CALPHAD award ceremony Presentation for the next CALPHAD meeting Conference dinner Korean traditional music performance

Thursday (Morning), May 27

Session 11 : CALPHAD approach related to ferrous alloys - I Chair : Qing Chen / Andre Schneider	
[O43] 08:30	*K. Ishida* α/γ equilibria and martensitic transformation in Fe-Mn-X(X: α stabilizing element) system
[O44] 08:50	*J.C. Rodríguez, L. Lozada, C. Tojal, T. Gómez-Acebo and F. Castro* Boron in steels. The Fe-Cr-B ternary phase diagram: application to liquid phase sintering of boron-containing stainless steels
[O45] 09:10	*Wei Xiong, Malin Selleby, Hualei Zhang and Levente Vitos* Remaining issues in the CALPHAD technique: Illustrations using the Fe-Cr and Fe-Ni binaries
[O46] 09:30	*Ikuo Ohnuma, Shinya Abe, Toshihiro Omori, Ryosuke Kainuma and Kiyohito Ishida* Experimental investigation and thermodynamic assessment of the Fe-Si binary system
[O47] 09:50	*Ales Kroupa, Dominik Legut, Jana Pavlu and A. Zemanova* The CALPHAD and *ab-Initio* modelling of Z-phase in ternary Cr-Nb-N system and advanced steels
10:10	Coffee Break (30min)
Session 12 : CALPHAD approach related to ferrous alloys - II Chair : K. Ishida / Ales Kroupa	
[O48] 10:40	*Philippe Schaffnit, Charles Stallybrass, Joachim Konrad and Axel Kulgemeyer* The CALPHAD approach in the development of micro-alloyed steels for line pipe applications
[O49] 11:00	*Qing Chen, Xiao-Gang Lu , Henrik Strandlund and Anders Engström* Modeling of metastable phase equilibria and phase transformations in multicomponent steels
[O50] 11:20	*Dong-Kwon Lee, Kyung-Jun Ko, Byeong-Joo Lee, Hyung-Ki Park and Nong-Moon Hwang* Monte-Carlo and phase field simulations of abnormal grain growth in Fe-3%Si steel approached by sub-boundary enhanced solid-state wetting
[O51] 11:40	*Chengying Tang, Minmin Tong, Yong Du, Honghui Xu, Joonho Lee, Qingrong Yao and Yuehui He* Phase equilibria of the Fe–Ni–Ta system at 1100 °C
[O52] 12:00	*Christian Leinenbach, Jiang Wang, Sebastian Buhl and Chunlei Liu* Interface reactions of Cu-Sn-Ti based active brazing filler metals with diamond and steel substrate
12:30	Lunch

Thursday (Afternoon), May 27

Session 13 : Database/software and CALPHAD approach related to metal-hydrogen system Chair : Bengt Hallstedt / S.R. Nishitani	
[O53] 14:00	*Suzana G. Fries, Mauro Palumbo, Thomas Hammerschmidt and Bo Sundman* The Sapiens project: a call for creating sustainable thermodynamic databases
[O54] 14:20	*Aimen Gheribi and Arthur D. Pelton* Identifying optimal conditions for alloy and process design using thermodynamic and properties databases, the FactSage software and the mesh adaptive direct searches algorithm
[O55] 14:40	*Bai Kewu and Wu Ping* Chemical potential phase diagrams and hydrogen storage thermodynamics
[O56] 15:00	*Ursula R. Kattner* Thermodynamic databases for metal-hydrogen systems
[O57] 15:20	*Jean-Marc Joubert and Stéphanie Thiébaut* Thermodynamic optimization of the system Pd-Rh-H-D-T
15:50	Coffee Break (30min)
Session 14 : CALPHAD approach related to thin films and phase field methods Chair : Suzana G. Fries / Wu Ping	
[O58] 16:20	*Bengt Hallstedt* Prediction of phase formation during thin film deposition by thermodynamic calculation
[O59] 16:40	*S.R. Nishitani, K. Togase1, Y. Tokumoto and I. Yonenaga* Micropipes and surface energy of compound semiconductors
[O60] 17:00	*M. Kajihara and M. Hashiba* Solid-state reactive diffusion in the Sn/(Pd-Ni) system
[O61] 17:20	*N. Moelans* Phase field simulations of growth and coarsening in the interdiffusion zone of leadfree solder joints
[O62] 17:40	*R.P. Shi, C.P. Wang, X.J. Liu and Y. Wang* Simultaneous mechanisms in the formation of core/shell microstructure
18:30	Dinner

Friday (Morning), May 28

Session 15 : Phase stability of alloy systems - I Chair : Hanchul Kim / Ursula R. Kattner	
[O63] 08:30	*Marcel H.F. Sluiter* Lattice stability in the presence of interstitial solutes
[O64] 08:50	*Tilmann Hickel, Ali Al-Zubi, Blazej Grabowski and Jörg Neugebauer* First principles determination of phase transitions in magnetic shape memory alloys
[O65] 09:10	*K. Santhy and K.C. Hari Kumar* Thermodynamic assessment of Nb-Ni-Ti ternary system by combining first-principles method and CALPHAD approach
[O66] 09:30	*Arkapol Saengdeejing, James E. Saal and Zi-Kui Liu* First-principles calculations and thermodynamic modeling of the B-C system
09:50	Coffee Break (30min)
Session 16 : Phase stability of alloy systems - II Chair : K. Santhy / Arkapol Saengdeejing (Awardees of the CALPHAD-STT Scholarship)	
[O67] 10:20	*Ji-Young Noh and Hanchul Kim* Electronic and elastic properties of $(Fe,Mn)_3AlC$ studied by density functional theory calculations
[O68] 10:40	*Jae Hoon Jang, In Gee Kim and H.K.D.H. Bhadeshia* Crystal structure and formation energy of epsilon-carbide
[O69] 11:00	*X. Tao, P. Jund, C. Colinet and J.C. Tédenac* Phase stability and physical properties of Cr_5B_3-type intermetallic compounds from first principles calculations
[O70] 11:20	*S. Ranganathan* Thermodynamic modelling of the non-equilibrium phase transformation during spontaneous vitrification in Ti-Cr alloys
11:40	Closing
12:00	Lunch

List of Poster Presentations (May 24 and 25)

[P1] *Honghui Xu, Biao Hu, Yong Du and Zhanpeng Jin*
Phase equilibria of the Ni-Si-Zn system at 600ºC

[P2] *Li Chen, She Q. Wang, Yong Du, Shu Z. Zhou, Tie Gang, Ji C. Fen, Ke K. Chang, Yi W. Li and Xiang Xiong*
Machining performance of Ti-Al-Si-N coated inserts

[P3] *Lijun Zhang, Yong Du and Ingo Steinbach*
Phase-field simulations of the Ni-Al diffusion couples

[P4] *Jianchuan Wang, Yong Du, Honghui Xu, Lixian Sun, Yi Kong, Chao Jiang and Yifang Ouyang*
The effect of Ti atom on hydrogenation of Al(111) surface

[P5] *Jingrui Zhao, Peisheng Wang, Hailin Chen, Yong Du, Lijun Zhang, Honhhui Xu and Shuhonh Liu*
Experimental investigation and thermodynamic modeling of the Cu-Fe-Mg and Cu-Mg-Si systems

[P6] *Weihua Sun, Yong Du, Honghui Xu and Zhaohui Yuan*
Experimental investigation and thermodynamic modeling on the Cu-Ni-Si system

[P7] *Jiang Wang, Christian Leinenbach and Chunlei Liu*
Development of the thermodynamic and atomic mobility database for active brazing of diamond to steel substrate

[P8] *Adela Zemanova and Ales Kroupa*
The experimental and theoretical study of the In-Ni-Sn system

[P9] *Luiz T.F. Eleno, Jacques Lacaze and Bo Sundman*
Thermodynamic assessment of the aluminum corner of the Al-Fe-M-Si system

[P10] *Luiz T.F. Eleno and Cláudio G. Schön*
The volume as a new variable in the cluster variation method (CVM)

[P11] *Nara M. Guimarães, Danieli A.P. Reis, Carlos de Moura Neto, Gilberto C. Coelho, Daniel S. de Almeida, Francisco Piorino and João M. Kruszy*
Experimental investigation of the ZrO_2-Y_2O_3-Nb_2O_5 system at 1550°C

[P12] *Satoshi Iikubo, Keisuke Tomiyasu, Kazumasa Horigane, Kazuyoshi Yamada, Hiroshi Ohtani and Mitsuhiro Hasebe*
Neutron diffraction study of $FeCr_2O_4$ spinel

[P13] *Leszek A. Zabdyr and Grzegorz Garzeł*
Assessment of the lead-free solder Bi-Cu-Sn alloy system.

[P14] *Nikolai M. Barbin, Dmitry I. Terentiev and Sergei G. Alekseev*
Thermodynamic simulation of oxidation of metal powders

[P15] *You Young Song, Seung-Woo Seo, In Gee Kim and H.K.D.H. Bhadeshia*
First-principles study on Fe substituted $Cr_{23}C_6$

[P16] *Kyoung-Won Park, Yoji Shibutani and Eric Fleury*
Packing structure and the permeation properties of hydrogen separable membrane in Ni-Al metallic glass

[P17] *Jaewon Chang, Sun-kyoung Seo and Hyuck Mo Lee*
Experimental investigation of phase equilibria in the Sn-Ni-Zn system

[P18] *Yi-Gil Cho*, *Hoon-Hwe Cho, Dong-Woo Suh, Jae Kon Lee and Heung Nam Han*
Numerical analysis of dilatational anisotropy of layered steel in dilatometry

[P19] *S. Jin, C. Leinenbach, J. Wang, A. Watson, A. Scott, S. Delsante and G. Borzone*
Experimental investigation and thermodynamic modeling of the Au-Ge-X (X=Cu, Ni) ternary systems

[P20] *Wan-Yi Kim, A. Nicholas Grundy, Eli Brosh, Eve Belisle, Christopher Bale, Arthur D. Pelton and Sergei A. Decterov*
A model and database for the viscosity of molten oxides

[P21] *Pertti Koukkari and Risto Pajarre*
Use of virtual invariant phases in rate-controlled Gibbs'ian calculations

[P22] *Y. Masaki, T. Ohshima, Y. Yamamoto, S.R. Nishitani and I. Yonenaga*
Stacking fault energy and structure energy difference of semiconductor compounds

[P23] *Reza Naraghi and Malin Selleby*
Thermodynamic re-assessment of the Iron-Carbon system

[P24] *Risto Pajarre, Pertti Koukkari and Toshihiro Tanaka*
Modeling the surface tension of reciprocal molten salt mixtures

[P25] *Joo Hyun Park*
Applications of computational thermodynamics on the phase equilibria of complex oxide systems for slags and inclusions in metallurgical industries

[P26] *Ji Hoon Ryu, Hyun You Kim, Da Hye Kim and Hyuck Mo Lee*
Amine induced structural change of cubo-octahedral platinum nanocluster and its properties

[P27] *Jae-Hyeok Shim, Ernst Kozeschnik, Woo-Sang Jung and Young Whan Cho*
Prediction of long-term precipitate evolution in austenitic heat-resistant stainless steels

[P28] *Kazuhisa Shobu*
CaTCalc - An advanced software for calculating thermodynamic equilibria and phase diagrams of multicomponent systems

[P29] *Chengying Tang, Tran Thai Bao, Joonho Lee and Yun-Mo Sung*
The melting of the silica–encapsulated silver nanoparticles

[P30] *R. Taniguchi, Y. Yamamoto, S.R. Nishitani and I. Yonenaga*
Local strains in SiGe alloys for the strained silicon

[P31] *K. Togase, S.R. Nishitani and T. Kaneko*
SiC polar surface energy by the first principles calculations

[P32] *T. Tokunaga, K. Yamada, S. Iikubo, H. Ohtani and M. Hasebe*
Thermodynamic analysis of phase equilibria in the Fe–Si–W ternary system

[P33] *Branislav Marković, Dragana Živković, Jan Vřešťál, Dragan Manasijević, Duško Minić, Nadežda Talijan and Radiša Todorović*
Experimental study and thermodynamic modeling of the Bi-Cu-Ni ternary system

[P34] *Wei-Wei Zhang, Ming Chen and Rasmus G. Barfod*
Thermodynamic Modeling of the CoO_x-FeO_y system

[P35] *J.J. Han, C.P. Wang and X.J. Liu*
A design method of Fe-based bulk metallic glass based on phase diagram calculation

[P36] *Risto Pajarre, Pertti Koukkari and Toshihiro Tanaka*
Modeling the effect of oxygen adsorption on surface tensions of molten metal alloys

[P37] *Y.C. Li, R.P. Shi, C.P. Wang, X.J. Liu and Y. Wang*
Predicting novel microstructures in polymer blends under two-step quench

[P38] *Y. Lu, C.P. Wang and X.J. Liu*
Phase diagram calculation of epitaxial $Pb(Zr_{1-x}Ti_x)O_3$ thin films at different thicknesses

[P39] *Z.S. Li, X.J. Liu and C.P. Wang*
Thermodynamic modeling of the Sn-U, Sn-Pu, Pb-U and Pb-Pu systems

[P40] *Y. Yu, C.P. Wang, X.J. Liu, R. Kainuma and K. Ishida*
Fcc-type miscibility gap in some Cu-Ni base alloys at high temperatures

[P41] *George Kaptay*
Theoretical derivation of the equation for the exponential temperature dependence of excess Gibbs energy of solutions

[P42] *Tran Thai Bao, Joonho Lee and Jung-Goo Lee*
Thermodynamic properties of Sn-Ag nanoparticles

[P43] *Taeyoung Kim, Eunju Kim, Joonho Lee and Youn-Bae Kang*
Using CALPHAD thermodynamic data to understand the carbothermic reduction of steelmaking slag by microwave heating

[P44] *Roberto R. de Avillez, André Costa e Silva and Raimundo A.F.O. Fortes*
Thermodynamic studies of steelmaking slags with respect to foaming in Electric Arc Furnace

[P45] *Ricardo N. Carvalho, Marilia M. Lima, Ricardo R. Silva, Cesar A.W. Olea, Marcelo A.C. Ferreira and André Costa e Silva*
Thermodynamic evaluation of the effects of segregation on phase transformations of 13Cr supermartensitic stainless steels

[P46] *Heung-Soon Lee and Byeong-Joo Lee*
Formation of Si/Ge bilayer nano-tubes by a self-bending process: A molecular dynamics study

[P47] *Daehoon Kang and In-Ho Jung*
Critical thermodynamic evaluation and optimization of the Ag-Zr, Cu-Zr and Ag-Cu-Zr systems and its applications to amorphous Cu-Zr-Ag Alloys

[P48] *Je-Wook Jang, Junhyun Kwon and Byeong-Joo Lee*
Effect of stress on self-diffusion in bcc Fe: An atomistic simulation study

[P49] *Hyun-Kyu Kim, Won-Seok Ko and Byeong-Joo Lee*
Atomistic modeling for NaCl-type MC carbides in steels

[P50] *Tae-Ho Lee, Chang-Seok Oh, Sung-Joon Kim and Eun-Joo Shin*
Experimental determination of stacking fault energy of the 18Cr-10Mn high interstitially alloyed stainless steels

[P51] *Alexander R. Abdulov, Pavel G. Agraval, Liya A. Dreval' and Mikhail A. Turchanin*
Thermodynamic assessments of the Cu–Ti–Zr system and boundary Cu–Ti, Cu–Zr, and Ti–Zr systems