

Report to 2008 APDIC

**Activities in 2007**  
**Korean Committee of Computational Materials Science and Engineering**  
**(formerly, Korean Committee of Thermodynamics and Phase Equilibria)**  
(Chairman: Dr. K.R. Lee at KIST)

Compiled by B.-J. Lee at POSTECH  
Presented by HM Lee at KAIST

**1. Phase Diagram Activities**

<p>Ex.PD = Experimental phase diagram study Ex.TD = Experimental study of thermodynamic data</p> <p>CA = Critical Assessment of literature TD Mod. = Thermodynamic Modeling, CALPHAD-type</p> <p>AS = Atomistic Simulations / First Principles</p> <p>Comment = notes on application etc., free text</p> <p>F = finished during 2007 X = work in progress</p>	<p><i>Contact Persons:</i></p> <p>Pak, J.-J. &lt;Hanyang Univ.&gt; &lt;jjpark@hanyang.ac.kr&gt; Jung, I.-H. &lt;RIST&gt; &lt;inho@rist.re.kr&gt; Lee, B.-J. &lt;POSTECH&gt; &lt;calphad@postech.ac.kr&gt; Lee, H. G. &lt;POSTECH&gt; &lt;hglee@postech.ac.kr&gt; Lee, H. M. &lt;KAIST&gt; &lt;hmlee@kaist.ac.kr&gt; Min, D. J. &lt;Yonsei Univ.&gt; &lt;chemical@yonsei.ac.kr&gt; Oh, C.-S. &lt;KIMM&gt; &lt;csoh@kims.re.kr&gt; Shim, J.-H. &lt;KIST&gt; &lt;jhshim@kist.re.kr&gt;</p>

System	Ex PD	Ex TD	CA	TD Md	AS	Comment	Contact person	Country
Al-Fe-N	F	F					Pak, J.-J.	KR
Al <sub>2</sub> O <sub>3</sub> -CaO-Fe <sub>t</sub> O-MgO-MnO-SiO <sub>2</sub>	F						Min, DJ	KR
B-C-Cr			X	X			Lee, B.-J.	KR
B-C-Fe			X	X			Lee, B.-J.	KR
B-C-Mo			X	X			Lee, B.-J.	KR
B-C-W			X	X			Lee, B.-J.	KR
Bi-Ni			F	F			Lee, HM	KR
Bi-Ni-Sn				F			Lee, HM	KR
C-Ti					X	MEAM interatomic potential	Lee, B.-J.	KR
CaO-MgO-MnO-SiO <sub>2</sub>	F						Min, DJ	KR
Cu-Fe-S			F	F			Lee, B.-J.	KR
Cu-Mn		F					Min, DJ	KR
Cu-S			F	F			Lee, B.-J.	KR
Cu-Ti					F	MEAM interatomic potential	Lee, B.-J.	KR
Cu-Zr					F	MEAM interatomic potential	Lee, B.-J.	KR
Fe-H					F	MEAM interatomic potential	Lee, B.-J.	KR
Fe-N-Ti	F	F					Pak, J.-J.	KR
Fe-O-Ti	F	F					Pak, J.-J.	KR
Ga-As					X	MEAM interatomic potential	Lee, B.-J.	KR
Ga-N					X	MEAM interatomic potential	Lee, B.-J.	KR
Ge					F	MEAM interatomic potential	Lee, B.-J.	KR
In					F	MEAM interatomic potential	Lee, B.-J.	KR
In-As					X	MEAM interatomic potential	Lee, B.-J.	KR
In-N					X	MEAM interatomic potential	Lee, B.-J.	KR
Mg					X	MEAM interatomic potential	Lee, B.-J.	KR
Mn					X	MEAM interatomic potential	Lee, B.-J.	KR
N-Ti					X	MEAM interatomic potential	Lee, B.-J.	KR
Si					F	MEAM interatomic potential	Lee, B.-J.	KR

## 2. Related Publications

### **Thermodynamics of Titanium and Oxygen Dissolved in Liquid Iron Equilibrated with Titanium Oxides**

Pak, JJ; Jo, JO; Kim, SI, et al., ISIJ INTERNATIONAL 47, 16-24 (2007)

### **Thermodynamics of Aluminum, Nitrogen and AlN Formation in Liquid Iron**

Kim, WY; Kang, JG; Park, CH, et al., ISIJ INTERNATIONAL 47, 945-954 (2007)

### **Thermodynamics of Titanium, Nitrogen and TiN formation in Liquid Iron**

Kim, WY; Jo, JO; Chung, TI, et al., ISIJ INTERNATIONAL 47, 1082-1089 (2007)

### **Activity Coefficient of Manganese in Copper**

Jung, SM; Rhee, CH; Min, DJ, ISIJ INTERNATIONAL 47, 1699-1701 (2007)

### **Solubility of MgO in Cao-SiO<sub>2</sub>-MnO Slags**

Jung, SM; Min, DJ; Rhee, CH, ISIJ INTERNATIONAL 47, 1823-1825 (2007)

### **Solubility of MgO in New Ironmaking Process-typed Slags**

Jung, SM; Min, DJ; Rhee, CH, ISIJ INTERNATIONAL 47, 1718-1722 (2007)

### **Thermodynamic Assessment of the Ni-Bi Binary System and Phase Equilibria of the Sn-Bi-Ni Ternary System,**

S. K. Seo, M. G. Cho, and H. M. Lee, Journal of Electronic Materials, Vols.36, 11 pp. 1536-1544 (2007)

### **Thermodynamic Calculations on the Stability of Cu<sub>2</sub>S in Low Carbon Steels**

Byeong-Joo Lee, Bo Sundman, Sung Il Kim and Kwang-Geun Chin, ISIJ International 47, 163 (2007).

### **A Semi-Empirical Interatomic Potential for the Cu-Ti Binary System**

Young-Min Kim, Byeong-Joo Lee, Materials Science and Engineering A 449-451, 733-736 (2007.03).

### **A Modified Embedded-Atom Method Interatomic Potential for the Cu-Zr System**

Young-Min Kim and Byeong-Joo Lee, J. Materials Research 23, 1095-1104 (2008.04).

### **A Modified Embedded-Atom Method Interatomic Potential for the Fe-H System**

Byeong-Joo Lee, Je-Wook Jang, Acta Materialia 55, 6779-6788 (2007.12).

**A Modified Embedded Atom Method Interatomic Potential for Indium**

Eun Cheol Do, Young-Han Shin, Byeong-Joo Lee, CALPHAD 32, 82-88 (2008.03).

**A Modified Embedded-Atom Method Interatomic Potential for Germanium**

Eun Ha Kim, Young-Han Shin, Byeong-Joo Lee, CALPHAD 32, 34-42 (2008.03).

### 3. Symposium on Computational Materials Science

#### 1) The Korean Institute of Metals and Materials, Computational Materials Science Subcommittee Symposium, Aug 16, 2007

**“First principles, Atomistic, Micro & Macro Scale Simulations” : 10 oral and 11 poster presentations**

**Abnormal Grain Growth of Goss Grains in Fe-3%Si Steel approached by Sub-Boundary Enhanced Solid-State Wetting**

Kyung Jun Ko, Pil Ryung Cha (Kookmin Univ.), Nong Moon Hwang, Seoul National Univ.

**Fractions of Grain Boundaries of High Mobility or Low Energy Necessary for Abnormal Grain Growth**

Dong Kwon Lee, Byeong Joo Lee (POSTECH), Nong Moon Hwang, Seoul National Univ.

**Thermal Fatigue Analysis of Copper via using 3D Discrete Dislocation Dynamics**

Gyu Seok Kim, Chan Seon Shin, Marc Fivel (CNRS), Kyu Hwan Oh, Heung Nam Han, Seoul National Univ.

**Study on Solid to Liquid Transition Region of the Ag-Pd Bimetallic Nanocluster through Collision**

Da Hye Kim, Hyun You Kim, Hyoung Gyu Kim, Ji Hoon Ryu, Hyuck Mo Lee, KAIST

**New Technique of Basin-Hopping Monte Carlo for Finding Global Optimization Structure of Nanoclusters**

Hyoung Gyu Kim, Hyun You Kim, Da Hye Kim, Ji Hoon Ryu, Hyuck Mo Lee, KAIST

**Collision and Surface Segregation in the Bimetallic Nanoclusters: Density Functional Theory and Molecular Dynamics Simulation**

Ji Hoon Ryu, Hyun You Kim, Hyoung Gyu Kim, Da Hye Kim, Hyuck Mo Lee, KAIST

**The Calculation of Elastic Constant for Fe with Temperature by Molecular Dynamics Simulation**

In Young Sa, Byung Joo Lee, POSTECH

**Modified Embedded Atom Method Interatomic Potentials for Germanium and Germanium-Silicon Binary system**

Eun Ha Kim, Young Han Shin, Byeong Joo Lee, POSTECH

**Effect of Size on the Phase Diagram of Small Particles: A Case Study of Ag-Au System**

Joong Chul Park, Joon Ho Lee, Korea Univ.

**Effects of Energy Dispersion of Incident Beams on Atomic Structure of Amorphous Carbon Films: Molecular Dynamics Simulation**

Kyung Soo Kim (Kookmin Univ.), Seung Chul Lee (KIST), Kwang Ryeol Lee (KIST), Pil Ryung Cha (Kookmin Univ.)

**A Theoretical Approach for Digestive Ripening**

Dong Kwon Lee (Seoul National Univ.), Sung Il Park (Samsung Advanced Institute of Technology), Jong K. Lee (Michigan Technological University Houghton), Nong Moon Hwang (Seoul National Univ.)

**Large Scale Three Dimensional Simulation of Ostwald Ripening**

Seong Gyoon Kim, Kunsan National Univ.

**Statistically Reliable EBSD Analysis method of Grain Boundary Characterization**

Dong-Ik Kim (KIST), Jun Yun Kang, Eun Kyu Her, Do Hyeon Kim, Se Jong Kim, Kyu Hwan Oh, Hu Chul Lee, Seoul National Univ.

**Effect of Strain on the Vacancy Formation of Ge: First-principles Approach**

Jung Hae Choi, Seung Chul Lee, Kwang Ryeol Lee, KIST

**Radiation Induced Hardening of Austenitic Stainless Steels: A Multiscale Modeling**

Chan Sun Shin, Jun Hyun Kwon, Korea Atomic Energy Research Institute

**in addition to 6 unlisted presentations**

**2) The 4<sup>th</sup> Conference of the Asian Consortium on Computational Materials Science (ACCMS-4),**

**Korea Institute of Science and Technology, Seoul, Korea, Sep 12 – 16, 2007**

210 researchers from 16 countries (not only in Asia but also in Europe and America) contributed 172 presentations in both oral (57) and poster (115) sessions.

9 technical sessions (Methodology, Future Materials for Energy, Nano-devices & Spintronics, Surface and Thin Films, Cluster, Nanotubes and Nanowires, Materials Structure Simulation, Oxide for Future Electronic Devices, Multiscale Approach for Industrial Applications, Nano-Bio System)

**3) The 6<sup>th</sup> Pacific Rim International Conference on Advanced Materials and Processing (PRICM-6), Jeju, Korea, Nov 5 – 9, 2007**

About 1200 researchers from 21 countries participated in 19 oral and 2 poster symposium.  
48 oral presentations (9 invited presentations) in the symposium of “Modeling and Simulation of Materials and Processes”.

## 4. MultiScale Computational Materials Design

