2011 APDIC Report

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ASM International

ASM Symposium at MS&T'10

- **Phase Stability, Diffusion Kinetics and Their Applications (PSDK-V)**
- Oral presentations (Appendix I) and a number of poster presentations.
- Organized by John E. Morral, Raymundo Arroyave, Yongho Sohn, Sudarsanam Babu, C. Robert Kao, and Jingxian Zhang.
- Sponsored by the ASM Alloy Phase Diagram Committee (Appendix II).
- The Gibbs Award recipients, Austin Chang (2009), and Arthur Pelton (2010) were honored during two special sessions of PSDK-V.

ASM Symposium at MS&T'11

- **Phase Stability, Diffusion Kinetics and Their Applications (PSDK-VI)**
- PSDK-VI will be held during the MS&T 2011 Conference & Exhibition in Columbus, Ohio, October 16-20, 2011.
- Organized by Jeffrey LaCombe, Raymundo Arroyave, John E. Morral, Weisheng Cao, Sudarsanam Babu, Yongho Sohn.
- Sponsored by the ASM Alloy Phase Diagram Committee.
- Special sessions are scheduled to honor the 2011 Gibbs Award recipient, John Cahn during the PSDK-VI symposium.

Miscellaneous

- Nominations for ASM Gibbs award have been solicited. 4 additional nominations were received.
- A recommendation for the 2012 recipient of the Gibbs Award has been forwarded to the ASM Board of Trustees.
- Papers selected from JPED/JPE/BAPD for a "Recommended Practices in Phase Diagram Evaluations" are accessible at the publisher's website, free of charge. (Appendix III).
- List of research on phase diagrams, first-principles calculations and kinetics has been compiled (Appendix IV).
- List of systems published in JPED from June 2010 to April 2011 has been compiled (Appendix V).

Appendix I

Materials Science and Technology 2010
Houston, TX, October 17-21, 2010

Phase Stability, Diffusion Kinetics, and Their Applications (PDSK-V)

Monday

Phase Field and Thermodynamic Modeling
Session Chairs: William Boettinger (NIST) and Yunzhi Wang (Ohio State University)

8:00 AM (Invited)
Phase Field Modeling of Beta to Alpha Transformations in Ti-6Al-4V (Invited)
Rongpie Shi and Yunzhi Wang (Ohio State University)
8:40 AM
Analysis of the Evolution of Complex Morphologies during Coarsening via Phase-Field Simulation
Chal Park[1], Katsuyo Thornton[1], and Peter W. Voorhees[2] ([1]University of Michigan; [2]Northwestern University)
9:00 AM
A Phase-Field Model for Precipitate Coarsening Kinetics in Ni Base Superalloys
Jingxian Zhang andAshish Patel (Carpenter Technology Corp.)
9:20 AM
Computational Modeling of Surface and Compositional Instabilities near a Free Surface
Andrew Boyne and Yunzhi Wang (Ohio State University)
9:40 AM Break
10:00 AM
Coring and Microstructural Evolution in Alloys
Patrice Turchi, James Belak, Jean-Luc Fattebert, Milo Dorr, Michael Wickett, Ming Tang, and Adam Schwartz (LLNL)
10:20 AM
Simulations of Interstitial Segregation on the Grain Boundary of B.C.C Metals: A Phase Field Approach Integrated with First-Principles Calculations
Kaisheng Wu, Michael Gao, Omer Dogan, and Paul King (National Energy Technology Lab)
10:40 AM
Effects of Impurities on the Grain Boundary Wetting and Penetration:
Kaveh Meshinchi Asl and Jian Luo (Clemson University)
11:00 AM
Thermodynamic Model of Hydride Formation and Dissolution in Spherical Particles
William Boettinger[1] and Yuri Mishin[2] ([1]NIST; [2]George Mason University)

Honorary Session: Honoring Y. Austin Chang, Recipient of ASM's 2009 J. Willard Gibbs Phase Equilibria Award
Session Chairs: Robert Kao (National Taiwan University) and J. C. Zhao (Ohio State University)

2:00 PM (Invited)
Integrated Computational Materials Engineering for Precipitation Simulation of Multi-Component Nickel and Aluminum Alloys
Y. Austin Chang (UW-Madison)
2:20 PM (Invited)
Calculation of Reaction Equations in Phase Diagrams
Shuanglin Chen[1], Ying Yang[1], Fan Zhang[1], Weisheng Cao[1], Rainer Schmid-Fetzer[2], and Y Austin Chang[3] ([1]CompuTherm, LLC; [2]TU Clausthal; [3]University of Wisconsin-Madison)
2:40 PM (Invited)
Application of Phase Diagram Calculation to Accelerated Development of Mo-Si-B Based Alloys

Ying Yang[1], H Bei[2], Shuanglin Chen[1], E George[2], J. Tiley[3], Y Chang[4] ([1]CompuTherm LLC; [2]ORNL; [3]AFRL; [4]University of Wisconsin-Madison)
3:00 PM (Invited)
Extracting Interdiffusion Coefficients from Multiphase Diffusion Couples:
Yuwen Cui and *Ji-Cheng Zhao* (Ohio State University)
3:20 AM Break
3:40 PM (Invited)
Applications of Equilibrium Phase Diagrams to Solving Materials Interactions Problems in Electronic Interconnects
*C. Robert Kao (*National Taiwan University)
4:20 PM (Invited)
Processing of Nanoscale Semiconductor Materials and Devices
Suzanne Mohney, Nicholas Dellas, Wenchong Ho, Bangzhi Liu, Sharis Minassin, Joan Redwing, and Theresa Mayer (Pennsylvania State University)
5:00 PM (Invited)
Unusual Phenomena Observed in Soldering: Understanding through Thermodynamics
Sinn-wen Chen, Hsin-jay Wu, Chih-ming Chen (National Tsing Hua University)

Tuesday

Diffusivity Modeling and Measurement
Session Chair: Yongho Sohn (University of Central Florida)

10:20 AM (Invited)
Modelling of Diffusion in Oxides and High-Temperature Oxidation
*John Agren (*Royal Institute of Technology)
11:00 AM
Diffusion Coefficients in Liquid Phase Predicted by ab initio Molecular Dynamics
Zi-Kui Liu[1], Xidong Hui[2], and Bill Wang[1] ([1]The Pennsylvania State University; [2]University of Science and Technology Beijing)
11:20 AM
Instrument Error and its Propagation through Diffusion Coefficient Measurement Procedures
Jeffrey LaCombe, and Alonso Jaques (University of Nevada)
11:40 AM
Self-Diffusion Studies in Magnesium Using Secondary Ion Mass Spectrometry
Nagraj Kulkarni[1], Peter Todd[2], Yong-ho Sohn[3], Sarah Brennan[3], Kevin Coffey[3], Mikhail Klimov[3], Graeme Murch[4], and Irina Belova[4] ([1]University of Tennessee/ORNL; [2]Oak Ridge National Laboratory; [3]University of Central Florida; [4]The University of Newcastle)

Diffusional Processes
Session Chair: John Agren (Royal Institute of Technology)

2:00 PM
Application of Computational Thermodynamics and Kinetics to Solid-State Joining of Advanced Materials
*Sudarsanam Babu (*Ohio State University)
2:20 PM
Simulations of Type 3 Boundaries Using the Dictra Homogenization Model
Xiaoqin Ke and John Morral (Ohio State University)
2:40 *PM*
Advanced Characterization of Microstructural Evolution in Titanium Copper Active Eutectoid System
Arun Devaraj[1], *Soumya Nag*[1], Rubens Caram[2], and Rajarshi Banerjee[2] ([1]Center for Advanced Research and Technology and University of North Texas; [2]University of Campinas)
3:00 PM
Evolution of Different Generations of Gamma Prime Precipitates in a Commercial Nickel Base Superalloy
Antariksh Singh[1], Junyeon Hwang[1], Soumya Nag[1], Rajagopalan Srinivasan[2], Jaimie Tiley[3], Babu Viswanathan3; Hamish Fraser[2], Rajarshi Banerjee[1] ([1]Center for Advanced Research and Technology and University of North

Texas; [2]Center for the Accelerated Maturation of Materials and Ohio State University; [3]Materials and Manufacturing Directorate, Air Force Research Laboratory)
3:20 PM
Effective Impurity Diffusion Investigation of Zr in Polycrystalline U-Mo at 550, 600, and 650°C
Ashley Ewh[1], Yongho Sohn[1], and Dennnis Keiser[2] ([1]Univ of Central Florida; [2]Idaho National Laboratory)
3:40 PM
Phase Stability and Low-Temperature Synthesis of Aluminide Coatings
Ridwan Sakidja and John Perepezko (University of Wisconsin-Madison)

Wednesday

Honorary Session: Honoring Arthur Pelton, Recipient of ASM's 2010 J. Willard Gibbs Phase Equilibria Award

Session Chairs: Gunnar Eriksson (RWTH Aachen University) and In-Ho Jung (McGill University)

8:00 AM (Invited)
The Geometry of General Phase Diagram Sections
*Arthur Pelton (*Ecole Polytechnique)
8:40 AM (Invited)
Applications of Thermodynamic Databases to Steelmaking Processes
*In-Ho Jung (*McGill University)
9:00 AM (Invited)
A Model and Database for the Viscosity of Molten Slags
Sergei Decterov,A. Grundy, Eli Brosh, Wan-Yi Kim, and Arthur Pelton (École Polytechnique de Montréal)
9:20 AM (Invited)
Using Thermochemistry to Solve Real-World Manufacturing Problems
*Susan Schiefelbein (*Corning)
9:40 AM Break
10:00 AM (Invited)
25 Years of Thermochemistry Applications
R. Diemer (DuPont Company)
10:20 AM (Invited)
Modeling the Thermodynamic Properties and Phase Equilibria in Molten Salt Systems: The Approach of Professor Arthur D. Pelton
*Patrice Chartrand (*Ecole Polytechnique)
10:40 AM (Invited)
Multicomponent Thermodynamic Database for the Mg Alloys Systems
Mamoun Medraj[1], Dmytro Kevorkov[1], Yinan Zhang[1], Mohammad Khan[1], and Mohammad Aljarrah[2] ([1]Concordia Univresity; [2]MTL – CANMET)
11:00 AM (Invited)
Thermodynamics of Iron at Extreme Conditions
Surendra Saxena[1], Gunnar Eriksson[2], and Suzana Fries[3] ([1]Florida Int University; [2]GTT; [3]Max Planck Inst Thermodynamic)
11:20 AM (Invited)
Thermodynamic Modelling: An Art or a Science?
Bo Sundman[1] and Suzana Fries[2] ([1]CEA; [2]Ruhr University Bochum)

Alloy Design and Phase Stability Modeling

Session Chairs: Raymundo Arroyave (Texas A&M University) and Zhang Jingxian (Carpenter Tech)

2:00 PM
CALPHAD Modeling of Hexagonal Laves Phases
Ursula Kattner (National Institute of Standards and Technology)
2:20 PM
Partition Behavior of Transition Metals in MX Carbide/Nitride and the Z-Phase: A First Principles Approach
Michael Gao, Chris Cowen, Paul Jablonski, and Jeff Hawk (NETL)
2:40 PM

Simulation of the Ferritic Nitriding Process - Database Development
Mei Yang[1], Danielle Belsito[1], Bo Yao[2], Yongho Sohn[2], and Richard Sisson[1] ([1]Worcester Polytechnic Institute, Center for Heat Treating Excellence; [2]University of Central Florida)
3:00 PM
Stability of Nanocrystalline Aluminum Grain Size in Cryomilled AA5083/ B4C Metal Matrix Composites
Travis Patterson[1], Clara Hofmeister[1], Bo Yao[1], Kyu Cho[2], Timothy Delahanty[3], and Yongho Sohn[1] ([1]University of Central Florida; [2]U.S. Army Research Laboratory; [3]Pittsburgh Materials Technology Incorporated)
3:20 PM Break
3:40 PM
Co_2NiGa Using First Principles
Avinash Chivukula, Ebubekir Dogan, Ibrahim Karaman, and Raymundo Arroyave (TAMU)
4:00 PM
Coupling Advanced Characterization with First-Principles Computations to Investigate Omega Precipitation in Titanium Alloys
Arun Devaraj[1], Soumya Nag[1], Robert Williams[2], Rajagopalan Srinivasan[2], Srinivasan Srivilliputhur[1], Hamish Fraser[2], and *Rajarshi Banerjee*[1] ([1]University of North Texas; [2]Ohio State University)

Thursday

Phase Stability and Diffusional Processes
Session Chair: John Morral (Ohio State University)

8:00 AM
High Temperature Phase Equlibrium of SiC-Si3N4-La2O3 System
Yuhong Chen, Zhenkun Huang, *Wenzhou Sun*, Yong Jiang, and Laner Wu (Beifang Ethnic University)
8:20 AM
Numerical Modeling for Magnetic Field Effects on Carbon Diffusion in Iron
Hiromichi Fujii[1], Toshimitsu Yokobori[1], and Sadahiro Tsurekawa[2] ([1]Tohoku University; [2]Kumamoto University)
8:40 AM
Influence of Grain Boundary Character on Point Defect Formation Energies in BCC Fe
Mark Tschopp[1], Mark Horstemeyer[1], Fei Gao[2], Xin Sun[2], and Moe Khaleel[2] ([1]Mississippi State University; [2]PNNL)
9:00 AM
Parameterization of the Reactive Force Field for Elastic Properties of Eucryptite Phases
Badri Narayanan[1], Adri van Duin[2], Branden Kappes[1], Cristian Ciobanu[1], and Ivar Reimanis[1] ([1]Colorado School of Mines; [2]The Pennsylvania State University)
9:20 AM
Kinetic Mass Diffusion Analysis to Predict Failure Mechanism of Interconnect Due to Electromigration
Yao Yao and Leon Keer (Northwestern University)
9:40 AM Break
10:00 AM
Investigation of the Hot Ductility Trough of Nb-Containing Low Alloy Steel
Jakob Six[1], Ali Göksenli[2], Sergiu Ilie[3], and Ernst Kozeschnik[1] ([1]Vienna University of Technology; [2]Istanbul Technical University; [3]Voestalpine Stahl Linz GmbH)
10:20 AM
Study of the β to γ Phase Transformation in High Nb Ti-Al-Nb Alloys
Sonalika Goyel, Michael Kesler, Ross Sacharow, and Fereshteh Ebrahimi (University of Florida)
10:40 AM
Precipitate in GTD-111 Ni-Base Superalloys
Mohammad Berahmand and Seyed Abdolkarim Sajjadi (Ferdowsi University of Mashhad)
11:00 AM
Modeling of Coarsening Behavior of γ' Precipitate in GTD-111 Ni-Base Superalloy
Mohammad Berahmand and Seyed Abdolkarim Sajjadi (Ferdowsi University of Mashhad)

Appendix II

Wednesday September 01, 2010

Alloy Phase Diagram Committee 2010-2011

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The Alloy Phase Diagram Committee oversees and guides ASM's involvement in alloy phase diagram data activities. It is responsible for monitoring the scopes of ASM and International Programs and ASM's input into those scopes, for monitoring the technical standards of ASM's products from these programs, for liaison with other alloy phase diagram committees, such as the International Commission on Alloy Phase Diagram Data. The Committee establishes policy related to the editorial content and scope of the Journal of Phase Equilibria and Diffusion, recommends approaches to serve and expand the subscriber and author base, and maintains continual surveillance of the technical quality of the publication. The Alloy Phase Diagram Committee shall support the ASM Strategic Plan and be accountable and responsible for those strategic actions which fall within the purview of the committee. It shall also be the responsibility of the committee to contribute new program and service ideas that support the Strategic Plan.

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Appendix III

Papers for Recommended Practice Guide: Phase Diagram Evaluations

Papers not subject to copyright:

A. Prince, "The critical assessment of ternary alloy phase diagram data," unpublished research with permission by S. Prince (2009).

E.R. Kreidler, "Standards for publication of phase equilibria studies," in "Applications of Phase Diagrams in Metallurgy and Ceramics Workshop Proceedings" Ed. G.C. Carter, NBS-SR 496, NBS, Gaithersburg, MD, pp. 1307-1324 (1977).

W.J. Boettinger, U.R. Kattner, K.-W. Moon and J.H. Perepezko, "DTA and heat-flux DSC measurements of alloy melting and freezing," SP 960-15, NIST, Gaithersburg, MD, (2007).

Non-BAPD/JPE/JPED papers recommended by Committee members (ASM-APDC or APDIC):

H.L. Lukas, E.-Th. Henig, and G. Petzow, "50 years reaction scheme after Erich Scheil," Z. Metallkd., 77 (1986) 360-367.

R. Schmid-Fetzer, D. Andersson, P.Y. Chevalier, L. Eleno, O. Fabrichnaya, U.R. Kattner, B. Sundman, C. Wang, A.Watson, L. Zabdyr and M. Zinkevich, "Assessment techniques, database design and software facilities for thermodynamics and diffusion," Calphad 31 (2007) 38-52.

R. Ferro, G. Borzone, G. Cacciamani and R. Raggio, "Calorimetric measurements in metallurgy: remarks on calibration and some specific problems," Thermochimica Acta 347 (2000) 103-122

R. Ferro, G. Cacciamani and G. Borzone, "Remarks about data reliability in experimental and computational alloy thermochemistry," Intermetallics 11 (2003) 1081-1094.

R. Ferro and A. Saccone, "Thermal analysis and alloy phase diagrams," Thermochimica Acta 418 (2004) 23-32.

T. Gödecke, "Ableitung des Kistallisationspfades in ternären Gusslegierungen (Derivation of the solidification path in ternary cast alloys)," Z. Metallkd. 92 (2001) 966-978. (in German)

Papers from BAPD, JPE, and JPED accessible on the web free of charge: all five papers are accessible at the following Springer web address: http://www.springer.com/materials/journal/11669?detailsPage=press

H. Okamoto and T.B. Massalski	"Guidelines for binary phase diagram assessment"	JPE 14, 316 (1993)	http://www.springerlink.com/content/100270622k03v066/
H. Okamoto and T.B Massalski	"Thermodynamically improbable phase diagrams"	JPE 12, 148 (1991)	http://www.springerlink.com/content/x19wr2456337m812/
R.D. Shull	"Phase diagram sample preparation"	BAPD 4, 5 (1983)	http://www.springerlink.com/content/q53203gxku637025/

D.A. Goodman, J.W. Cahn and L.H. Bennett	"The centennial of the Gibbs-Konovalov rule for congruent points: Its underlying theoretical basis and its application to phase diagram evaluation"	BAPD 2, 29 (1981)	http://www.springerlink.com/content/d313454034nx8n34/
J. Zhao and M.R. Notis	"Phase transformation kinetics and the assessment of equilibrium and metastable states"	JPE 14, 303 (1993)	http://www.springerlink.com/content/q8143j81231660tg/

Other suggested papers from BAPD, JPE, and JPED:

S.M. Allen and J.W. Cahn	"Phase diagram features associated with multicritical points in alloy systems"	BAPD 3, 287 (1982)
G. Inden	"The effect of continuous transformations on phase diagrams"	BAPD 2, 412 (1981)
Y.T. Zhu, J.H. Devletian and A. Manthiram	"Application of differential thermal analysis to solid-solid transitions in phase diagram determination"	JPE 15, 37 (1994)
J.W. Cahn	"Obtaining inferences about relative stability and metastable phase sequences from phase diagrams"	BAPD 1, 27 (1980)
N. A. Gokcen and Z. Moser	"Thermodynamics of phase equilibria"	JPE 14, 288 (1993)
A.D. Romig, Jr.	"Thermodynamic considerations in the analysis of phase stability: The role of interfacial equilibrium in the determination of phase diagrams by x-ray microanalytical techniques"	BAPD 8, 308 (1987)
O.N. Carlson and J.F. Smith	"Effects of interstitial impurities on phase equilibria"	BAPD 8, 208 (1987)
J.W. Herchenroeder and K.A. Gschneidner	"Stable, metastable and nonexistent allotropes"	BAPD 9, 2 (1988)
J.F. Smith	"Crystallography and phase equilibria a review: Part III-Second-order transitions and approximations"	JPED 26, 5 (2005)
J.F. Smith	"Crystallography and phase equilibria a review: Part I-Basics"	JPED 25, 405 (2004)
V. Raghavan and D.P. Antia	"Pressure variable, phase rule, and phase diagram: A tutorial"	JPE 19, 101 (1998)
A.P. Miodownik	"The effect of magnetic transformations on phase diagrams"	BAPD 2, 406 (1981)
M. Hillert and J. F. Smith	"The shape of solidus and liquidus curves"	BAPD 4, 361 (1983)
R.G. Connell	"A tutorial on flow diagrams: A tool for developing the structure of multicomponent phase diagrams"	JPE 15, 6 (1994)

V. Raghavan and D.P. Antia	"Adjoining phase regions on two-dimensional phase diagrams: A tutorial"	JPE 21, 121 (2000)
J.F. Smith, K.J. Lee and D.M. Bailey	"Resolution of conflicting data: I. Temperature and Equilibrium"	BAPD 5, 133 (1984)
W.C. Johnson and P.W. Vorhees	"Coherent Phase Diagrams"	BAPD 9, 208 (1988)
A. Prince	"To speculate or not to speculate"	BAPD 2, 149 (1981)
J.F. Smith	"Crystallography and phase equilibria a review: Part II-Space groups and structure"	JPED 25, 497 (2004)
N. Kanani and K. Loehberg	"Nomenclature and geometrical representation of invariant phase equilibria in multicomponent systems"	BAPD 5, 229 (1984)
D.E. Peterson	"Disturbance of equilibria by decay of radioactive components"	BAPD 8, 203 (1987)

BAPD=Bulletin of Alloy Phase Diagrams
JPE=Journal of Phase Equilibria
JPED=Journal of Phase Equilibria and Diffusion

Appendix IV

Report to APDIC, May 2011
Phase Diagram Activities in U.S.A.

Report compiled by: Patrice Turchi and Yongho Sohn, 11-May-2011

From the 30 researchers contacted regarding their activities in phase diagram research, 11 responses were received from:

Raymundo Arroyave	<rarroyave@tamu.edu>
Saurabh Bajaj	<saurabh_02@neo.tamu.edu>
Carelyn E. Campbell	<carelyn.campbell@nist.gov>
Albert V. Davydov	<albert.davydov@nist.gov>
Ursula R. Kattner	<ursula.kattner@nist.gov>
Zi-Kui Liu	<dr.liu@psu.edu>
John E. Morral	<morral.4@osu.edu>
Philip Nash	<nash@iit.edu>
John H. Perepezko	<perepezk@engr.wisc.edu>
Yongho H. Sohn	<ysohn@mail.ucf.edu>
Patrice E.A. Turchi	<turchi1@llnl.gov>

Keys for Table:

Ex.PD	= Experimental phase diagram study
Ex.TD	= Experimental study of thermodynamic data
CA	= Computational Atomistics
CT	= Computational Thermodynamics
ICE	= Intellectual Critical Evaluation of all Experimental Data
Kin	= Kinetic Studies
Comment	= notes on application etc.,

F = finished in 2009 or 2010
X = work in progress

System	Ex PD	Ex TD	CA	CT	ICE	Kin	Comment	Contact Person
Au-O-Zn	X			X	X		Preliminary assessment	Davydov A.V.
B-Li				F	F			Kattner, U.R.
B-Ca-H				F	F			Kattner, U.R.
B-Ca-H-Li-Mg-Si					F			Kattner, U.R.
Cr-Ni-Ti-Zr				X	X			Kattner, U.R.
Mn-Ni-Ti-Zr				X	X			Kattner, U.R.
Co-Fe-O				X	X	X		Kattner, U.R. with C.E. Campbell
Ni-Re	X			X	X			Kattner, U.R. with J.H. Perepezko
Cu-In-Se						X		Campbell C.E.
Cu-Ga						X		Campbell C.E.
Ni-X (Al,			X	X	X		F-P of coefficient of	Liu, Z.K.

Co, Cr, Cu, Fe, Hf, Mo, Nb, Pt, Re, Ta, Ti, W, Y and Zr)							thermal expansions	
Ni3Al+X (Cr, Hf, Pt, Y and Zr)			X	X	X		F-P of coefficient of thermal expansions	Liu, Z.K.
Al-Pt			F	F	F		F-P and thermodynamic modeling, published	Liu, Z.K.
Ni-Al-Pt			F	X	X		F-P and thermodynamic modeling	Liu, Z.K.
Co-Pt			F	F	F		F-P and thermodynamic modeling, submitted	Liu, Z.K.
TGO in Ni-Al base alloy					X		working on manuscript	Liu, Z.K.
B-C	F	F		F	F		First draft of the B-C manuscript is send to all the co-authors	Liu, Z.K.
Mg-B-C			F	F	F		Optimization is done. Manuscript is in process	Liu, Z.K.
X doped MgB2			F		F		Calculations are done. Manuscript is in process	Liu, Z.K.
Cu-Hf	F	F	F	F	F		F-P for all compounds in the system, send F-P part of the Cu-Hf manuscript to Yu Zhong	Liu, Z.K.
Hf-Cu-Ni		X			X		Outline for the experimental paper, Preliminary database, preliminary liquid optimization	Liu, Z.K.
Al-Mn			F	F			Phonon & Thermodynamics for compounds by F-P (Published in Comput. Mater. Sci.)	Liu, Z.K.
Ni-Pt			F	F			Phonon & thermodynamics for ordered and disordered phases by F-P + SQS (Published in PRB)	Liu, Z.K.
Ti			F	F		F	Diffusion coefficients by F-P calculations (submitted, under review)	Liu, Z.K.
Ni			X	X			Stacking fault energy and shear strength in (111) plane by F-P	Liu, Z.K.
Ni-X			X	X			Stacking fault energy affected with 24 X elements by F-P	Liu, Z.K.
Ce-Sn and Mg-Ce-Sn			X	F	F		F-P for all compounds in the binary system+CALPHAD modeling combining the published database	Liu, Z.K.
Sn-Sr and Mg-Sn-Sr			X	X	F		F-P for all compounds in the binary system+CALPHAD modeling combining the	Liu, Z.K.

							published database	
Mg2SiO4-Mn2SiO4			X	X	F		F-P for the two endmembers in the pseudobinary system, Mg battery	Liu, Z.K.
Re-Y			F	F	F		Published in Intermetallics, 2010	Liu, Z.K.
Re-Ti			F	X	F		FP hcp.bcc SQS, Debye model	Liu, Z.K.
Ni-Re				F	F		re-modeled with Pure 4, published in Intermetallics, 2010	Liu, Z.K.
Ni-Re-Y				F	F		Published in Intermetallics, 2010	Liu, Z.K.
Mg-Al	F		F				elastic constants of Al12Mg17 and pure elements by diffusion couples, submitted to Scripta Mat	Liu, Z.K.
Ca-Ce-Mg	X						diffusion couple investigation	Liu, Z.K.
Mg-Zn	X						diffusion couple investigation	Liu, Z.K.
Hf-W	F	F		X			Hf-W phase diagram assesment with FP input including SQS, finite temperature assesment with Debye model	Liu, Z.K.
Fe-W	F	F		X			existing model in PBIN uses old desciptions for liquid phases, will re-model; FP 0K calculations	Liu, Z.K.
Ti			F	F			Thermodynamics and pressure-temperature phase diagram by first-principles calculations	Liu, Z.K.
BiMnO3 and BiFeO3			F	F			Pressure-Temperature phase diagram by first-principles calculations and CALPHAD	Liu, Z.K.
TiO2			F	F			Thermodynamics and pressure-temperature phase diagram by first-principles calculations	Liu, Z.K.
PbTiO3			F	F			Thermodynamics and pressure-temperature phase diagram by first-principles calculations	Liu, Z.K.
BaO-TiO2				X			Pseudobinary refinement	Liu, Z.K.
La2O3-TiO2				X			Pseudobinary preliminary modeling	Liu, Z.K.
SrTiO3			F				Phonons	Liu, Z.K.
Sr2RuO4			F				Phonons	Liu, Z.K.
Al2O3			F				Phonons and Thermodynamics	Liu, Z.K.
MgO			F				Phonons	Liu, Z.K.
h-BN			F				Phonons	Liu, Z.K.
BaFe2As2			F				Phonon, spin, and Fermi surface	Liu, Z.K.
BiFeO3			F				Phonons and	Liu, Z.K.

							Thermodynamics	
MnO and NiO			F				Phonons and LO-TO spliting	Liu, Z.K.
SiC			F				Phonons	Liu, Z.K.
Mg			F				Stacking fault	Liu, Z.K.
Sr-Co-O			X	X	F		Thermodynamic modeling of perovskite and neighboring phases	Liu, Z.K.
La-Sr-Co-O			X	X	F		Thermodynamic modeling of perovskite and neighboring phases	Liu, Z.K.
Al-Ni						F	Structure, diffusivity and viscosity in liquid state	Liu, Z.K.
Al-Zr						F	Structure, diffusivity and viscosity in liquid state	Liu, Z.K.
Al-Cu						F	Structure, diffusivity and viscosity in liquid state	Liu, Z.K.
Ni-W						X	Structure, diffusivity and viscosity in liquid state, GB energy and mobility	Liu, Z.K.
Zr-Re				X	X		Zr-Re phase diagram modeling	Liu, Z.K.
Mg-X (X=Y, Zn, Fe and Al)						X	Stacking fault energy	Liu, Z.K.
Li-X-B-H (X=Mg,Ca, and Zn)			F	F	F		Published in International Journal of hydrogen energy, 2010	Liu, Z.K.
Cs-In			F	F	F		Published in CALPHAD, 2010	Liu, Z.K.
La-Ca-Fe-O			X	F	F		Thermodynamic modeling of perovskite and neighboring phases	Liu, Z.K.
Hf-Re	F	F		X			FP for all compouunds, bcc and hcp SQS, CALPHAD modeling	Liu, Z.K.
M3C (M=Co, Cr, Fe, Hf, Mn, Nb, Ni, Mo, Si, Ta, W)			F	F			Phase stability, finite temperature thermodynamics, elastic properties, and electronic structure of M3C with the structure of cementite	G. Ghosh
U-Zr			X	X	X	X	Normal and radiation damage conditions	Morral, JE
Am-Pu			F	F			Am-Pu phase diagram assessment with input from ab initio: Mansucript submitted to JNM	Turchi, P.E.A.
Mo-U			X	X			Manuscript submitted to J. of Nucl. Mater.	Turchi, P.E.A.
Ta-U			X	X				Turchi, P.E.A.
Pu-V			F	X				Turchi, P.E.A.
Pu-Ta			F	X				Turchi, P.E.A.
Pu-W			F	X				Turchi, P.E.A.
U-W			F	X				Turchi, P.E.A.
Am-Np				F			Am-Np phase diagram assessment	Turchi, P.E.A.
Am-U				F			Am-U phase diagram assessment	Turchi, P.E.A.

Pu-U			F				Pu-U studied by ab initio. JNM408, 61-66 (2011)	Turchi, P.E.A., Landa, A.I., Söderlind, P.
Np-Pu			F				Pu-U studied by ab initio. JNM408, 61-66 (2011)	Turchi, P.E.A., Landa, A.I., Söderlind, P.
Cm-Pu			F				Pu-U studied by ab initio. JNM408, 61-66 (2011)	Turchi, P.E.A., Landa, A.I., Söderlind, P.
Np-Zr			F	F			Np-Zr phase diagram assessment with input from ab initio:JNM409, 1-8 (2011)	Bajaj, S., Garay, A., Landa, A., Söderlind, P., Turchi, P.E.A., Arroyave, R.
Ti-U			F	F			Mo-Ti phase diagram assessment with input from ab initio: Mansucript submitted to JNM	Bajaj, S., Landa, A., Söderlind, P., Turchi, P.E.A., Arroyave, R.
Be-Cu-Fe-Nb-Ta-Ti-Zr				X			Database development	Turchi, P.E.A., Lordi, V., Kaufman, L.
Mo-Ta								Perepezko, J. and Turchi, P.E.A,
Mo-Si-B-C						X		Perepezko, J.
Ga-Ni				X			Ga-Ni phase diagram assessment	Arroyave, R.
Fe2YZ (Y=TM, Z=III-V)	X	X	X	X			collaboration with Yong Du	Nash, P.
Ni2YZ (Y=TM, Z=III-V)	X	X	X	X			collaboration with Yong Du	Nash, P.
Co2YZ (Y=TM, Z=III-V)	X	X	X	X			collaboration with Yong Du	Nash, P.
Ag-Mg	X	X					B2 phase	Nash, P.
Ag-Mg-In	X	X					B2/L21	Nash, P.
Ti-Al-Ru	X	X					Isothermal section at 1200C	Nash, P.
Bi-In-Sn-Ga	X			X				Nash, P.
U-Mo	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Mo-Al	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Mo-Al-Si	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Mo-Nb	F					F	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Mo-Ti	F					F	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Nb-Zr	F					F	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Fe	F					F	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Fe-Cr	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Fe-Ni-Cr	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Zr-Fe	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Zr-Fe-Cr	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Zr-Fe-Ni-Cr	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
U-Mo-Zr	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.

U-Mo-Nb	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Mg-Al	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Mg-Zn	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Mg-Y	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Mg-Nd	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Mg-Gd	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Mg-Al-Zn	X					X	Phase diagram and diffusion coefficients	Sohn, Y.H.
Ni-Al-Ta						F	Diffusion in Ni3Al	Sohn, Y.H.
Ni-Al-Re						F	Diffusion in Ni3Al	Sohn, Y.H.
Ni-Al-Ir						F	Diffusion in Ni3Al	Sohn, Y.H.

Appendix V

Journal of Phase Equilibria and Diffusion
Published from June 2010 to April 2011

Evaluations

Ag-Pb-Te	Au-Ba-Ge	Fe-Sr	Mo-Y	Sr-V
Al-C-O-Si-Y	B-Nb-Si	Mn-B	Ni-P	V-RE
Al-Hf-Zr	Fe-Cr	Mn-Sr	Ni-Sr	
Al-Nd-Zr	Fe-Nb	Mo-Ce	Sr-Ti	

Ternary and Higher Order Iron and Aluminum Phase Diagram Updates

Ag-Al-Cu-Mg	Al-Cu-Gd	Al-Ir-Ni	C-Fe-N-Ti	Fe-O-Sn
Al-Au-Cu	Al-Cu-Ir	Al-Ir-Ru	Co-Cr-Si	Fe-O-Zn
Al-B-Mg	Al-Cu-Li	Al-La-Sb	Co-Nb-Si	Fe-Mg-Ni-O
Al-Bi-Si	Al-Cu-Sc	Al-Mg-Si-Zn	Co-Ni-Y	Fe-Ni-Si-Zn
Al-C-Co	Al-Er-Fe	Al-Mg-Sn	Co-Sn-Zr	Fe-O-Si-Zn
Al-Ca-Mg	Al-Er-V	Al-Mg-Zn	Cr-Fe-Y	Fe-O-Sn-Zn
Al-Ce-Cu	Al-Eu-Zn	Al-Mo-Ti	Cr-Hf-Ni	Fe-Sb-Zn
Al-Ce-Zr	Al-Fe-Nb	Al-Nb-Ti	Cr-Ni-Re	Fe-Tb-V
Al-Co-Fe	Al-Fe-Ni	Al-Ni-Pt	Fe-Ga-Nd	Fe-Ti-Zr
Al-Cr-Fe-Zn	Al-Fe-Ni-O	Al-P-Zn	Fe-Gd-Ti	Mo-Ni-Re
Al-Cr-Ni	Al-Fe-O	Al-Pr-Zr	Fe-Mg-O	Nb-Ni-Re
Al-Cr-Pd	Al-Fe-O-Zn	Al-Sb-Si	Fe-Mn-S	Ni-Re-V
Al-Cr-Ti	Al-Fe-Si	Al-Si-V	Fe-Nb-V	Ni-Re-Ti
Al-Cu-Dy	Al-Fe-Si-Zn	Al-Y-Zr	Fe-Nb-Zn	
Al-Cu-Er	Al-Fe-Zn	Bi-Fe-Ni-Zn	Fe-Ni-O	
Al-Cu-Fe	Al-Fe-Zr	Bi-Fe-Sn	Fe-Ni-Ta	

Supplemental Literature Review

Al-Mo	Cl-F	Dy-Ti	La-Zn	Pr-Zn
Al-Ta	Cl-O	Eu-F	Mg-Pd	S-Sm
As-I	Cl-Re	F-Xe	Mg-Sb	Sb-Y
Ba-Li	Cl-W	Ga-Ni	Mn-S	Sc-Th
Bi-Ti	Co-Sm	H-Na	Mo-Re	Si-V
Bi-Tm	Co-Zr	H-Ti	Mo-Si	Sn-Zr
C-Cl	Cr-Ge	Hf-I	Ni-Pt	V-W
Ca-Sr	Cu-Li	I-Pb	P-Te	
Ce-Pt	Dy-Mn	I-Sb	P-Zn	