CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: CALPHAD XXXIII—An International Conference on Phase Diagram Calculations and Computational Thermochemistry
AI No. 20.06002.01.081.325; Account No. 20.06002.01.081

DATE/PLACE: May 31–June 4, 2004, Krakow, Poland

AUTHOR: Yi-Ming Pan

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SUBJECT:	CALPHAD XXXIII—An International Conference on Phase Diagram Calculations and Computational Thermochemistry
DATE/PLACE:	May 31–June 4, 2004, Krakow, Poland
AUTHOR:	Yi-Ming Pan [Center for Nuclear Waste Regulatory Analyses (CNWRA)]
PERSONS PRESENT:	Yi-Ming Pan (CNWRA) and approximately 150 participants from 30 countries.

BACKGROUND AND PURPOSE OF TRIP:

The CALPHAD (an acronym for the Calculation of Phase Diagrams) annual conference is an international forum that gathers worldwide experts for a review of the current status of the computational thermodynamics development and promotes international collaboration. The main goals of the CNWRA staff attending the 2004 conference were to present a paper on issue related to Alloy 22 phase stability and to keep current worldwide advancements in computational thermodynamics.

SUMMARY OF PERTINENT POINTS:

The CALPHAD XXXIII conference had 19 sessions in the areas of CALPHAD calculations and modeling, first-principles (*ab initio*) calculations, experimental studies of alloys and nonmetallic systems, diffusion and kinetics, soldering materials and databases, and industrial applications. About 160 papers were presented in oral and poster sessions. I made an oral presentation of the paper co-authored by D. Dunn and G. Cragnolino and titled Phase Stability of Alloy 22 High-Level Waste Container Weldments: Experiments and Thermodynamic Calculations. The paper discussed results of recent work investigating the effects of fabrication processes on the material stability of Alloy 22, focusing on the evaluation of compositional variations and thermomechanical treatments using thermodynamic calculations. Participation in this conference enabled staff to present to the international community the methodology used to assess the DOE model approach and predictions of the long-term stability of Alloy 22. It was also beneficial to engage in discussion on the first-principles computational methodology that is currently being developed by the staff for computing thermodynamic data for long-range ordering in Alloy 22. A number of pertinent papers are summarized in this report.

T.B. Massalski (Carnegie Mellon University) opened the technical sessions with a plenary lecture on The Complex World of Plutonium Science, discussing the most unusual metallurgical, electronic, and nuclear properties of plutonium. The peculiar nature of the transition between bonding and localization of the 5f electrons that occurs at plutonium leads to many complex electronic interactions and physical properties. The metallurgical challenges for engineering applications of plutonium are particularly great because of its phase instability with temperature, pressure, and chemical additions. The retention of the δ-phase of plutonium with the addition of a few percent gallium or aluminum was discussed on the basis of the United States and Russian versions of the Pu-Ga phase diagram. While the Russian phase diagram represents the equilibrium condition, the U.S. phase diagram is in fact the metastable condition but an adequate working diagram because the kinetics of the δ-phase decomposition are very slow.

Z.K. Liu (Pennsylvania State University) presented a talk CALPHAD Modeling: What More Can Be Done? and pointed to two main concerns in current practice of CALPHAD modeling—lack of experimental data for new materials and reliability of the predictions. The modeling of Gibbs energy of individual phases and the coupling of phase equilibria and thermochemistry are the key in developing internally consistent thermodynamic descriptions of multicomponent systems. Thermochemical data, such as enthalpy and entropy of formation, obtained from first-principles calculations were discussed. Integration of the calculated first-principles data with the existing experimental data into CALPHAD modeling improves its predictive power.

B. Sundman (Royal Institute of Technology, Sweden) discussed Phase Transformations with Fast Diffusing Elements for simulating solidification of steels with a significant fraction of interstitial elements. An alternative model has been implemented in Thermo-Calc to allow carbon to redistribute between solid and liquid phases during solidification. The results obtained from this study showed better agreement with experimental data in comparison with those from Scheil and DICTRA simulations.

L. Kaufman (MIT) gave a review presentation titled The CALPHAD Approach to Computational Thermodynamics that focused on current practice where computational thermodynamics methods are used with success. Since computational thermodynamics applies the results of measurements and observations, made under conditions where equilibrium prevails, to commercial practice where nonequilibrium or quasi-equilibrium persists, computational thermodynamics must have a broader scope than used in classical thermodynamics. The success achieved by pursuing this track is the explicit description of the stability of unstable and metastable phases and the functional descriptions of the compositional, temperature, and pressure dependance of the Gibbs energies and entropies of such phases. Among several examples of recent work presented, the talk touched on application of Thermo-Calc software to calculation of Pourbaix diagrams for Alloy 22 in predicting formation of oxides. Comparison of the calculated oxide phases formed in simulated groundwaters with the experimental data showed some are good and some are poor.

H. Ipser (University Wien, Austria) gave an invited talk titled COST 531—A European Action on Lead-free Soldering. COST, founded in 1971, is an intergovernmental framework for European Co-operation in the field of Scientific and Technical Research. It has almost 200 Actions and involves the participation from 34 European member countries and 11 outside EU, non-member countries. The COST 531 Action on lead-free soldering is structures into four Working Groups: WG1 on thermodynamic database and phase diagram information, WG2 on theoretical modeling, WG3/4 on physical and chemical properties, and WG5/6 concerned with reliability, processing, and packaging issues. Currently 9 Group Projects are active involving 38 participating research institutions from 15 European countries. The Action has identified nine quaternary systems for a lead-free solder thermodynamic database, comprising five ternary solder alloys with relevant substrate materials. The ultimate goal is no lead in electrical and electronic equipment in Europe from July 1, 2006.

K. Tanaka (Toyota Central R&D Labs., Inc.) presented a paper titled Application of CALPHAD Method to Design a Cost Effective and Productive Heat-resistant Iron Alloys. The objective of this development work was to lower the material cost by replacing a cast product made of Inconel 713C nickel-base superalloy with iron-base alloys with comparable strength at 650–750 °C. Using Thermo-Calc and Ni-alloy database, a new heat resistant iron-base alloy has been designed and optimized to have a desirable strength at elevated temperatures.

Special attention has been paid to balance the amount of strengthening precipitates and brittle σ-phase, and to ensure the castability in the atmosphere by the addition of niobium.

In the poster titled Phase Equilibria in Ni-Al-Cr-Co-W-Re System: Modeling and Experiments, J. Bursik (Academy of Science of the Czech Republic) discussed methods of modeling phase equilibria and kinetics of ordering processes in Ni-based superalloys. The Monte Carlo approach in combination with first-principles calculations were used. Complementary calculations of phase diagrams were also run with Thermo-Calc software. The predictions showed reasonably good agreement with the experimentally observed microstructures by means of analytical scanning and transmission electron microscopy.

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

CONCLUSIONS/RECOMMENDATIONS:

The CALPHAD conference provided excellent opportunities to keep current with the worldwide advancements in computational thermodynamics, and to interact with scientists, particularly from Europe where a broader international joint effort in this rapidly expanding field remains strong. Participation in this conference promoted international interaction and collaboration, and provided an excellent avenue to keep up with the latest advances in emerging computational thermodynamics and applications. These international interactions enhance the U.S. Nuclear Regulatory Commission (NRC)/CNWRA capability for the resolution of key technical issues, and make NRC/CNWRA activities and decisions more effective, efficient, and realistic through the acceptance of international experts. Future participation in the CALPHAD conferences is highly recommended.

REFERENCES:

The conference program with the meeting agenda and the list of the papers is included as an attachment to this trip report. A book of conference abstracts and list of participants was published by the organizers and is available from the author upon request.

SIGNATURES:

Yi-Ming Pan
Senior Research Engineer

6/25/04
Date

CONCURRENCE:

Vijay Jain, Manager
Corrosion Science and Process Engineering

6/25/04
Date

Budhi Sagar
Technical Director

6/25/04
Date

ATTACHMENT

Monday, May 31

8:00 to 19:00		**Registration at the Conference Office** The Jagiellonian University - Collegium Medicum 12 St. Anna's Str.
8:30		**Opening and Welcome Addresses**
SESSION 1 **CALPHAD CALCULATIONS AND MODELLING** **Chairman: MOHRI Tetsuo** **Room: Aula**		
9:00	1.1 Plenary Lecture	MASSALSKI Thaddeus B. and HECKER S. S. *The Complex World of Plutonium Science*
9:40	1.2 Invited Lecture	DECTEROV Sergei A., JUNG I.-H., JAK E., KANG Y.-B. and PELTON A. D. *Thermodynamic Modeling of Oxide Systems*
10:10	1.3 Invited Lecture	GACHON Jean-Claude *Experimental Determination of Phase Diagram. Classical and Non Classical Methods*
10:40		**Coffee Break**

SESSION 1 (continuation) **CALPHAD CALCULATIONS AND MODELLING** **Chairman: ISHIDA Kiyohito** **Room: Aula**		
11:10	1.4	CAO W., CHANG Y. Austin, ZHU J., CHEN S.-L. and OATES W. A *Application of the Cluster/site Approximation to the Calculation of Multicomponent Alloy Phase Diagrams*
11:30	1.5	SCHILLE J.-P., MIODOWNIK A. Peter., SAUNDERS N. and GUO Zhanli *The Thermodynamics of Deformation Martensite*
11:50	1.6	VITEK John M., MASIASZ P. J. and KLUEH R. L. *Comparison of Predicted and Measured Phase Stability of Precipitates in Cr-Mo Steels*
12:10	1.7	UDOVSKY Alexander L. *Covariant Form of the System of Equations for Two-phase Equilibria and its Application for Creation of the General Method of Clculation of Tie-line in Multi-component Systems*
12:30	1.8	GRUNDY A. Nicholas, HALLSTEDT B., and GAUCKLER L J. *Assessment of the La-Sr-Mn-O System and the Defect Chemistry of (La, Sr)MnO_3 Perovskites*
12:50	1.9	ROÓSZ Andras, KAPTAY G. *ESTPHAD – A New and Fast Way to Reproduce the Results of CALPHAD Calculations During Simulation of Phase Transformations*
13:10		**Lunch (Restaurant "Wierzynek")**

SESSION 2 **CALPHAD CALCULATIONS AND MODELLING** **Chairman: SCHMID-FETZER Rainer** **Room: Aula**		
14:25	**Announcment :** **The Best Paper Award of APDIC at the Calphad XXXIII Conference**	
14:30	2.1	LIU Zi-Kui *CALPHAD Modeling: What More Can Be Done?*
14:50	2.2	OHTANI Hiroshi, YAMANO M. and HASEBE M. *Thermodynamic Analysis of the Co-Al-C and Ni-Al-C Systems by Incorporating Ab Initio Energetic Calculations into the CALPHAD Approach*
15:10	2.3	SÜSS Rainer, CORNISH L., GLATZEL U. *Comparison of Experimentally Determined and CALPHAD - determined Results of the Pt-Cr-Ru System*
15:30	2.4	KOBERTZ D., HILPERT K., KAPAŁA J., MILLER Mirosław *Phase diagram, thermodynamic activities and thermodynamic modelling in the NaBr-DyBr3 system*
15:50	2.5	SUNDMAN Bo, CHEN Qing *Phase Transformations with Fast Diffusing Elements*
16:10	2.6	GOLCZEWSKI Jerzy A. and ALDINGER F. *Thermodynamic Modelling of Polymer Precursor Derived Amorphous Si-C-N Ceramics*
16:30	**Coffee Break**	

	SESSION 2 (continuation) **CALPHAD CALCULATIONS AND MODELLING** **Chairman: KOZUBSKI Rafał** **Room: Aula**		**SESSION 3** **EXPERIMENTAL STUDIES** **Chairman: TEDENAC Jean-Claude** **Room: Asklepiosa**	
17:00	2.7	ASP Klara and ÅGREN J. *CALPHAD and Phase-field Simulations of Sintering*	3.1	TENG Lidong, LU X., AUNE R. E., and SEETHARAMAN S. *Thermodynamic Studies of Cr3C2 and Reassessment of Cr-C System*
17:20	2.8	HALLSTEDT Bengt and SCHNEIDER Jochen M. *A Simple Approach to Pressure Dependence, Examplified in the Al-Mg-Si System*	3.2	TANASESCU Speranta, MARINESCU C., MAXIM F. *Contributions to Electrochemical Determination of Phase Diagrams and Thermodynamic Characterization of the Perovskite-Type Compounds in La-Mn-O System*

17:40	2.9	MASUDA-JINDO K., HUNG Vu Van and KIKUCHI R. *First Principles Computations of Alloy Phase Diagrams by Statistical Moment and Cluster Variation Methods*	3.3	DU Yong, SCHUSTER J. C., HUANG B.Y.1, XU H.H., and JIN Z.P. *Phase Equilibria of the Al-Mn-Si System over the Entire Composition and Temperature Ranges: Modeling and Experiment*
18:00	2.10	WALDNER Peter *Thermodynamic Modelling of High-Temperature Heazlewoodite*	3.4	SZTUBA Z. , MUCHA I. , GAWEŁ Wieslaw, ZALESKA E. Thermal Analysis of the Tl2Se– Bi2Se3 System
18:20	2.11	ABRIKOSOV Igor A. *First-principles Simulations of Alloy Thermodynamics at High Pressure*	3.5	TOKUNAGA Tatsuya, OHTANI H. and HASEBE M. Thermodynamic Evaluation of Phase Equilibria and Glass Forming Ability in the Fe-Si-B System
19:00	**Dinner (Restaurant "Wierzynek")**			

Tuesday, June 1

SESSION 4
CALPHAD APPROACH TO COMPUTATIONAL THERMODYNAMICS

Chairman: MIODOWNIK Peter
Room: Aula

9:00	4.1 Plenary Lecture	KAUFMAN Larry *(Ct) The Calphad Approach To Computational Thermodynamics*
9:40	4.2 Invited Lecture	SCHMID-FETZER Rainer, GRÖBNER J. and MIRKOVIC D. *Constitution, Grain Refining and Solidification Enthalpies of Al-Ce-Si Alloys*
10:10	4.3 Invited Lecture	KOZUBSKI Rafal, KOZŁOWSKI M., PARTYKA E., PIERRON-BOHNES V., PFEILER W. *Vacancy Thermodynamics and the Kinetics of Superstructureformation in Intermetallic Compounds*
10:40	**Coffee Break**	

	SESSION 5 DIFFUSION AND KINETICS **Chairman: SUNDMAN Bo** **Room: Aula**		SESSION 6 EXPERIMENT AND MODELLING **Chairman: KOZUBSKI Rafal** **Room: Asklepiosa**	
11:10	5.1	MIYAZAKI Toru, KOZAKAI T. and SCHOEN C. G. *The Kinetics of Precipitate-Nucleation in the Edge of Miscibility Gap.*	6.1	ZAKHAROV A.Yu., ZAKHAROV Maxim A., UDOVSKY A.L., OONK H. *Statistical Thermodynamics of Binary Systems with Variable Valent States (Mixed Valence) of Ions for One of Components. Application for the Uranium-Oxygen System*
11:30	5.2	JANCZAK-RUSCH J., KLOCH , J., GUZIK E., WOLCZYNSKI Waldemar *Phenomenon of Back-diffusion in Formation of Intermetallic Structure Within Ni/Al/Ni Interconnection*	6.2	UDOVSKY Alexander L., YSTINOVSHIKOV, Yu.I.,PUSHKAREVB.E. *Application of Thermodynamic Approach for Press Down on Formation of Brittle Sigma-Phase in Fe-Cr Alloys: Computer Design and Experiment*
11:50	5.3	SCHNEIDER André, ZHANG J., BERNST R., INDEN G. *Thermodynamics and Kinetics of Phase Transformations During Metal Dusting of Iron and Iron-based Alloys*	6.3	BLUM M., GERK M., GLAUM Robert, ÖZALP D., and SCHMIDT A. *Redox Equilibria Between Phosphates And Phosphides In Phase Diagrams M / P / O (M = Cr, Mn, Co, Ni, Cu)*

12:10	5.4	STRANDLUND Henrik and LARSSON H. *Computer Simulations of the Kirkendall Effect in Binary and Multicomponent Alloys*	6.4	JANOVEC Josef, JENKO M. and HOMOLOVA V. *Practical Aspects of Thermodynamic Calculations*
12:30	5.5	GUY Bernard *Aqueous Saturation and Precipitation\ Dissolution Kinetics of Solid Solutions Discussed by Use of Chemical Potential Phase Diagrams*	6.5	FRISK Karin *Thermodynamic Modelling of Multicomponent Systems*
12:50	5.6	INDEN Gerhard, SCHNEIDER A. *DICTRA Simulation of Precipitation Reactions in Ferritic Steels*	6.6	ONG W.P., DU Yong, HUANG B.Y., SCHMID-FETZER R., ZHANG Q.F., XU H.H. *Thermodynamic Reassessment of the Al-V System*
13:10		**Lunch (Restaurant "Wierzynek")**		

	SESSION 7 EXPERIMENT Chairman: KAPTAY Gyorgy Room: Aula		SESSION 8 MODELLING Chairman: CHANG Y. Austin Room: Asklepiosa	
14:30	7.1	YAZHENSKIKH Elena, WILLENBORG W., HACK K., MUELLER M.,HILPERT K., SINGHEISER L. *Alkali Pressures over Sodium Aluminosilicates: Comparison of Experimental Data and Thermodynamic Calculations*	8.1	HU S.Y., VAITHYANATHAN V., LIU Z.K., CHEN L.Q., MURRAY Joanne L., WANG W., WEILAND H. *Modeling Precipitate Microstructure Evolution in Al-Cu Alloys*
14:50	7.2	ZABDYR Leszek A. and FABRICHNAYA O. B. *Phase Equilibria in the Co-Cu-Si-O System*	8.2	MARKUS Torsten, HILPERT K. *Chemical Transport of Alumina in metal halide lamps - Thermodynamic Modelling and experimental data*
15:10	7.3	AURELIO Gabriela, GUILLERMET Fernández A., CUELLO G.J. *Structural Properties, Relative Stability and High Temperature Reactions of Metastable Phases in Zr-Nb and Ti-V Alloys*	8.3	OHNUMA Ikuo, KAMIYA N., KAINUMA R. and ISHIDA K. *Experimental Investigation and Thermodynamic Assessment of the Interaction between the Chemical and Magnetic Ordering of the Fe-Al and Fe-Ga systems*
15:30	7.4	ZAKULSKI Wojciech *Thermodynamics of the Al-Mg-Sr liquid solutions*	8.4	LEE Byeong-Joo *Computation of Grain Boundary Energy byA Semi-Empirical Atomistic Approach*
15:50	7.5	MEDRAJ Mamoun *Thermodynamic Modeling and Experimental Investigation of the Equilibria in Mg-Al-(Ca, Sr, Sb)*	8.5	SHANG Shunli, BÖTTGER A. J. *The gamma-Fe[N] /gamma'-Fe4N1-x Phase Equilibrium: a Combined Statistical Thermodynamic and Ab Initio Calculations Approach*

16:10	7.6	BROŻ Pawel., BURŠIK J., PICHA R. and ŠIMEČEK J. *Modelling and Experimental Study of Phase Equilibria in Ni-Al-Cr-Ti and Ni--Al-Cr-Co Systems*	8.6	BROSH Eli, MAKOV Guy , SHNECK Roni Z. *Equations of State for Modelling of High-Pressure Equilibria*
16:30 to 18:00		**Coffee break & Poster session I**		
17:40		**New software presentations**		
19:00		**Dinner (Restaurant "Wierzynek")**		

Wednesday, June 2

SESSION 9 **AB INITIO CALCULATIONS** **Chairman: IPSER Herbert** **Room: Aula**		
9:00	9.1 Plenary Lecture	MOHRI Tetsuo, CHEN Y. and OHNO M. First-principles Calculation of Phase Equilibria and Extension to Hybridized Calculation with Phase Field Method
9:40	9.2 Invited Lecture	VŘEŠŤÁL Jan., KROUPA A. and ŠOB M. Application of AB Initio Electronic Structure Calculations in Calphad Method
10:10	9.3	DE FONTAINE Didier, OZOLINS V., ISLAM Z., MOSS S. First Principles Calculations of Oxygen Ordering in the YBCO Superconductor
10:30	**Coffee break**	
SESSION 10 **AB INITIO CALCULATIONS** **Chairman: DE FONTAINE Didier** **Room: Aula**		
11:00	10.1	HOUSEROVÁ Jana., VŘEŠŤÁL J. and ŠOB M. Modelling the Sigma Phase in the Mo-based Systems Using Ab Initio Electronic Structure Calculations
11:20	10.2	NISHITANI Shigeto R., SEKO A., YUGE K. and ADACHI H. First Principles Prediction on Cluster Free Energy of Precipitate Nucleation
11:40	10.3	CHEN Ying, IWATA S. and MOHRI T. Analytical Structure of the Cluster Expansion Method and Some Applications to Fe Based Phases Equilibria
12:00	10.4	ANDERSSON David Ab Initio Based Modeling of Titanium Compounds Having Defect Lattices
12:20	10.5	BALUN Jozef, HOUSEROVA J., KROUPA A., INDEN G. The Modelling of Important Intermetallic Phases, Existing in Fe-based Systems by the Combined CALPHAD and Ab-Initio Approach
12:40	**Lunch (Restaurant "Wierzynek")**	
14:00	**Tour to Wieliczka Salt Mine**	
20:00	**Banquet (Restaurant "Cracovia")**	

Thursday, June 3

	SESSION 11 **EXPERIMENTAL STUDIES AND SOLDERING MATERIALS** **Chairman: MOSER Zbigniew** **Room: Aula**	
9:00	11.1 Plenary Lecture	ISHIDA Kiyohito *Development of Advanced Materials Based on Phase Diagrams and Microstructural Control*
9:40	11.2 Invited Lecture	IPSER Herbert *COST 531 - A European Action on Lead-free Soldering*
10:10	11.3 Invited Lecture	MOSER Zbigniew, GĄSIOR W., ISHIDA K., OHNUMA I., BUKAT K., PSTRUŚ J., SITEK J. and KISIEL R. *Eperimental Wettability Studies Combined with the Related Properties from Data Bases for Lead-free Soldering Materials*
10:40	**Coffee break**	

	SESSION 12 **SOLDERING MATERIALS** **Chairman: GACHON Jean-Claude** **Room: Aula**		**SESSION 13** **EXPERIMENT, MODELLING** **Chairman: WOLCZYNSKI Waldemar** **Room: Asklepiosa**	
11:10	12.1	KIM Jong Hoon and LEE Hyuck Mo *Application of Multicomponent Phase Diagrams in Understanding Phase Evolution of the Solder/UBM Systems*	13.1	JOUBERT Jean-Marc, SUNDMAN B. and DUPIN N. *Reassessment of the niobium-nickel system using site occupancy parameters for the μ phase*
11:30	12.2	VIZDAL Jiri, KROUPA A., POPOVIC J., ZEMANOVA A. *Experimental and Theoretical Study of Phase Equilibria in Sn-Zn-X (X = Bi, In, Pd) systems*	13.2	BONNET Frédéric, LEHMANN J., GAYE H. *General Description of the Liquid Steels by the "Central Atoms" Model*
11:50	12.3	GARZEŁ G., ZABDYR Leszek A. and ONDERKA B. *Phase Equilibria in the Ag-Bi-Sn Lead-free Solder Alloys*	13.3	WANG Chong, ZINKEVICH M., FABRICHNAYA O., ALDINGER F. *Experimental Investigation and Thermodynamic Modeling on the ZrO2-GdO1.5 System*

12:10	12.4	KAPTAY Gyorgy *Modifications to the Butler Equation (Calculating the Surface Tension of Liquid Alloys from Bulk Thermodynamic Properties)*	13.4	PETERSEN Stephan *Process Modelling Applications with SimuSage*
12:30	12.5	KAPTAY G., ZIVKOVIC Dragana, BUDAI I. *Estimation of Viscosity for Binary and TernaryLiquid Alloys in the Cu-Au-Ag System from Thermodynamic Data, Using a NewTheoretical Approach*	13.5	JEPPSSON Johan and ÅGREN J. *Modelling of the Temporal Evolution of Particle Size Distributions in Crystalline Solids*
12:50	12.6	ZAJACZKOWSKI Andrzej, BOTOR J. *Thermodynamics of the In-Sb System and Gaseous Phase of Antimony Determined by Vapour Pressure Measurements*	13.6	KUCHARSKI Marian, FIMA P. *The Surface Tension and Density of Cu-Pb-Fe Alloys*
13:10		**Lunch (Restaurant "Wierzynek")**		

	SESSION 14 DATA BASES Chairman: CHEN Ying Room: Aula		SESSION 15 EXPERIMENT AND MODELLING Chairman: LEE Byeong-Joo Room: Asklepiosa	
14:30	14.1	DINSDALE Alan T. *SGTE and the Development of Thermodynamic Databases*	15.1	SU X. and TEDENAC Jean-Claude *Thermodynamic Modeling of the Cobalt-Gallium System*
14:50	14.2	PICHA R., VŘEŠŤÁL Jan, KROUPA A. *Prediction of Surface Tension of Alloys Based on Thermodynamic and Thermophysical Data*	15.2	COSTA E SILVA Andre, AVILLEZ R., BENEDUCE F. *A Preliminary Evaluation of Selected TiO2 Containing Oxide Systemswith Applications in Slag-Steel-Inclusion Equilibria*
15:10	14.3	ZINKEVICH Matvei, GEUPEL S., SOLAK N., ALDINGER F. *Development of the Thermodynamic Database for the System La-Sr-Ga-Mg--Ni-O*	15.3	PAN Yi-Ming, DUNN D.S. and CRAGNOLINO G.A. *Phase Stability of Alloy 22 High-Level Waste Container Weldments: Experiments and Thermodynamic Calculations*
15:30	14.4	ROBELIN Christian, CHARTRAND P. and PELTON A. D. *A Thermodynamic Database for AlCl3-based Molten Salt Systems*	15.4	NOVAKOVIC Rada and RICCI E. *Surface and Transport Properties of Al-Ti Liquid Alloys*
15:50	14.5	LU Xiaogang, SELLEBY M. and SUNDMAN Bo *Theoretical Approach in Developing a Molar Volume Database*	15.5	GUMIŃSKI Cezary Peculiarities of the Binary Phase Diagrams with Alkali Metals

16:10	14.6	FABRICHNAYA Olga., WANG Ch., LAKIZA S.,ZINKEVICH M.,ALDINGER F. *The Thermodynamic Description of the Ternary Systems ZrO2-Gd2O3-Al2O3, ZrO2-Gd2O3-Y2O3 and Gd2O3-Y2O3-Al2O3.*	15.6	BALANETSKYY S., GRUSHKO B., KOWALSKA-STRZĘCIWILK E., VELIKANOVA Tamara Ya., URBAN K. *Investigation of the Al-Pd-Fe Alloy System*
16:30	14.7	GĄSIOR Władysław, MOSER Z., DĘBSKI A. *Database of Physical Properties of the Lead-free Solder Materials*	15.7	CHEN Ming, HALLSTEDT B., and GAUCKLER L. J. *Thermodynamic Assessment of the Mn-Y-Zr-O System*
16:50 to 18:20		**Coffee break & Poster session II**		
17:50		**New software presentation**		
19:00		**Dinner (Restaurant "Hawelka")**		

Friday, June 4

	SESSION 16 APPLICATIONS Chairman: FITZNER Krzysztof Room: Aula	
9:00	16.1 Plenary Lecture	HILPERT Klaus Thermodynamic Data of Intermetallics by Mass Spectrometric Vaporisation Studies
9:40	16.2 Invited Lecture	FITZNER Krzysztof Application of Chemical Thermodynamics in Industrial Silver Production Process
10:10	**Introduction to Calphad 2005**	
10:30	**Presentation of Calphad - journal**	
10:40	**Coffee break**	
	SESSION 17 APPLICATIONS Chairman: VRESTAL Jan Room: Aula	
11:10	17.1	MICZKOWSKI Zdzisław, CZERNECKI J Blister Copper Production at Polish Smelters
11:30	17.2	IWANCIW Jerzy The Coefficients of Regular Solution Model for Steelmaking Slags
11:50	17.3	AVILLEZ Roberto R. and COSTA E SILVA A. L.V. A Preliminary Evaluation of the Fe Rich Region of the Fe-Nb-P System and its Implications on the Processing of IF (Interstitial Free) Steels
12:10	17.4	TANAKA Kouji, KAWAURA Hiroyuki, NISHINO Kazuaki Application of CALPHAD Method to Design a Cost Effective and Productive Heat-Resistant Iron Alloys
12:30	17.5	GÓMEZ-ACEBO Tomas, Ortiz P. and Castro F. Thermodynamic Analysis of the Gas-Solid Interaction During Sintering of Cr-containing P/M Steels

12:50	17.6	KALICKA Z., KAWECKA-CEBULA E. and WYPARTOWICZ Jan The Solubility of Sulphur in Oxide Inclusions in Silicon Steel
13:10	**Closing ceremony**	
13:20	**Lunch (Restaurant "Wierzynek")**	
Departure		

Poster Session I

Tuesday 1 June 16:30

The Jagiellonian University - Collegium Medicum
12 St. Anna's Str.

PI-1 GRÖBNER Joachim, MIRKOVIC D. and SCHMID-FETZER R.
Thermodynamic Approach in Grain Refinement of Al-Si Alloys Using Ti and B

PI-2 SEIFERT Hans-Jurgen, WAGNER S., ULLMANN T., ALDINGER F.
Thermodynamic Compatibility of Yttrium Silicate Coatings with CVD-SiC Coated C/C-SiC Materials

PI-3 KAPAŁA Jan
Management Program for BINGSS Phase Diagram Optimizer

PI-4 URBANIK Witold., KAPAŁA Jan., ZNAMIEROWSKA T.
Thermochemistry of the Pseudobinary $NaPO_3 - Na_4P_2O_7$ system

PI-5 VASSILEV Gueorgui Penev, RADEVA K. I.
Phase Equilibria in the Zn-rich Regions of the Cu-Ni-Zn and Co-Ni-Zn Systems

PI-6 VASSILEV Gueorgui Penev
Phase Formation in the System Ti-Sn-Si

PI-7 DOBREV Evgueni S., VASSILEV G.P., TEDENAC J-C
Experimental Study of the System Sn-Ti-Zn to 600°C

PI-8 VASSILEV G. P., DOBREV Evgueni S. TEDENAC J.-C.
Study of the Phase Equilibria in the Ag-Sn-In System at 280°C

PI-9 KLOTZ Ulrich E.
Building a Thermodynamic Database for Active Brazing Metals

PI-10 WOJEWODA Joanna, ZIĘBA P., SANDERS S.
Phase Characterization in the Cu/In-Bi 22at.%/Cu Interconnections

PI-11 ZEMANOVÁ Adela, , VŘEŠŤÁL J., SEMENOVA O., IPSER H., KROUPA A.
Prediction of Phase Equilibria in the Ag-In-Pd System in Comparison with Experimental Data

PI-12 NIEVA N.,ARIAS Delia Ernestina
New Results in the Experimental Study of the Zr-Sn-Fe Phase Diagram. 800 and 900°C Isothermal Sections

PI-13 RAMOS C., SARAGOVI C.,ARIAS Delia Ernestina, GRANOVSKY M.
New Experimental Results on the Ternary Zr-Nb-Fe System

PI-14 GRANOVSKY M. S., MAINARDI D. and ARIAS Delia Ernestina
Experimentals results related to the Zr-Fe phase diagram

PI-15 MATSUMIYA Tooru, SAITO K., KANEHASHI K. and YAMADA W.
A Proposal for the Development of Thermodynamic Model of Refining Slag

PI-16 KIM Young-Min, LEE J., LEE B.-J.
Semi-empirical Atomic Potentials for Ti and Zr

PI-17 HALLSTRÖM Samuel, LU X. and ÅGREN J.
Thermodynamic Assessments of the Ni-Al-Ru and Ni-Al-Pt Systems and Optimization of Mobilities

PI-18 RAUNO Luoma
A Thermodynamic Analysis of the System Fe-Cr-Ni-C-O

PI-19 ANTONI-ZDZIOBEK Annie and DURAND-CHARRE M.
Phase Relationships in the Iron-rich Region of the Ternary System Fe-W-C

PI-20 ZIVKOVIC Dragana, MANASIJEVIC D., ZIVKOVIC Z.
Thermodynamic Study of the Ag-In-Sb System

PI-21 KOSTOV A.,ZIVKOVIC Dragana, ZIVKOVIC Z.
Thermodynamics and Characterization of Alloys in Ga-Ge-Sb System

PI-22 MENDE Tamás, ROÓSZ András
Calculation of the Equilibrium Phase Diagram of Ca-Mgo-Al2O3-SiO2 Ceramic System by the ESTPHAD Method

PI-23 PAN Z., DU Yong, HUNAG B.Y., XU H.H. and SCHMID-FETZER R.
Experimental Investigation and Thermodynamic Modeling of the Al-Be-Si Ternary System

PI-24 COSTA E SILVA Andre, RIZZO F. and SPEER J. G.
A Study of the Partition of Elements Between Austenite and Ferrite in Condition Similar to the treatment of TRIP Steels

PI-25 LEE Jinwook, KIM Y.-M., LEE B.-J.
Semi Empirical Atomic Potential of Carbon

PI-26 IKHSANOV Renat Sh., UDOVSKY A.L.
Jacobi Matrix and Generalized Van der Waals Equations Set for m-phase n-component Equilibrium

PI-27 ZALESKA Ewa., MUCHA I., GAWEŁ W.
Re-examination of the $Tl_2Te - In_2Te_3$ System by Electrochemical Method

PI-28 RZYMAN Krzysztof., MOSER Z., GACHON J-C.
Calorimetric Studies of the Enthalpies of Formation of Al_3Ti, Al_2Ti, $AlTi$, $AlTi_3$ Compounds.

PI-29 ALSAEED Rashed A.
Thermodynamics of Gold-Calcium Alloys

PI-30 ABBASOV Almuk S., ALIYEV I.Y., SULEYMANOV Z.I., ASKEROVA K.A., ALIYEVA N.A., BAGIROVA S.D.
The Phase Equilibrium and Thermodynamic Properties of Cu(Ag) – Ga(In) – S(Se, Te) Systems

Poster Session II

Thursday 3 June 16:50

The Jagiellonian University - Collegium Medicum
12 St. Anna's Str.

PII-1 BUCHTOVÁ Veronika, VŘEŠŤÁL J., KROUPA A.
Comparison of Theoretical Calculations of Phase Equilibria in The System Ag-In-Sb with Experimental Data

PII-2 GLAUM Robert, TRAPPE O. and BLUM M.
The Computer Program Cvtrans and its Application to Modeling of Chemical Vapour Transport Experiments with Transition Metal Phosphides

PII-3 KJELLQVIST Lina
Assessment of Iron-Ruthenium

PII-4 CACCIAMANI Gabriele, WATSON A., PARODI N., PATRONE M., BORZONE G., FERRO R.
Experiments and Modelling of Lead-free Solder Alloys: Preliminary Results on the Au-In-Sn System

PII-5 GEMME Frédéric
Application of the Quasichemical Model for Multicomponent Systems on the Calculation of Volumetric Properties for liquid Aluminum Alloys

PII-6 VAN DE WALLE A., MOSER Zbigniew and GĄSIOR W.
First-principles Calculation of the Phase Diagram of Cu-Li System

PII-7 KISSAVOS Andreas, SHALLCROSS S., MEDED V., KAUFMAN L., and ABRIKOSOV I. A.
First-principles Calculations of Mixing Enthalpies in Mo-Ru System

PII-8 KAPALA Jan, RUTKOWSKA I.
Thermodynamic Properties of the Pseudobinary $CsCl$-$LnCl_3$ (Ln = lanthanide) Systems

PII-9 YAGHMAEE M. S., DEMETER Zsolt, KAPTAY G..
Measurement of Mixing Enthalpy in Liquid Binary KCl-K_2TiF_6 System

PII-10 BUDAI Istvan, BENKŐ M.Z., KAPTAY G.
Modelling Concentration Dependence of Surface Tension and Viscosity of the Ag-Sb Liquid Alloy from Thermodynamic Data

PII-11 FARKAS Janos, ROÓSZ A.
Treatment of Al-Mg-Si Ternary Phase Diagram by ESTPHAD method

PII-12 KÖVÉR Z., ROÓSZ András
Calculation of the Equilibrium Phase Diagram of Fe-C Alloy System by the ESTPHAD Method

PII-13 WATSON Andy, SCOTT A., HOUSEROVA J., VŘEŠŤÁL J.
Thermodynamic Assessment of the Bi-Pd System

PII-14 AURELIO Gabriela, BOZZANO P.B., GUILLERMET Fernández A., CUELLO G.J.
High Temperature Reactions of Metastable Phases in Zr-Nb Alloys

PII-15 GUMIŃSKI Cezary
Binary Phase Diagrams of Mercury and the Priodic Tble of Eements

PII-16 SEKO Atsuto, NISHITANI S. R., TANAKA I. and ADACHI H.
Applications of the First Principles Prediction for Precipiatate Nucleation Free Energy on Ternary and Highly Strained Systems

PII-17 HANSEN S., JANZ Andreas , GRÖBNER J. and SCHMID-FETZER R.
Thermodynamic Modeling of Bi-Sn-Hg Alloys

PII-18 SCHMID-FETZER Rainer and JANZ A.
Impact of Ternary Parameters

PII-19 DU Yong, CHANG Y. A. and HUANG B. Y.
Microstructure and Microsegregation in Multicomponent Al-356 Alloys: Directional Solidification Experiment and Modeling

PII-20 CHEN H., DU Yong, XU H.H., HUANG B.Y. , XIONG W., PAN Z., and SCHUSTER J. C.
Reassessment of the Nb-Ni System: Key Experiment and Thermodynamic Modeling

PII-21 XIONG W., DU Yong, GONG W.P., LIU Y., XU H.H., HUANG B.Y., CHEN H.L., PAN Z.
Thermodynamic Assessment of the Mo-Nb-Ta System

PII-22 WANG X., TEDENAC Jean-Cloud, SU X. and YIN F.
A thermodynamic Assessment of the Dy–Sn System

PII-23 GHANBARI Ahari K. , THOMPSON D., ARGENT B.B. and SHARP J.H.
Recent Progress in the Prediction of the Phase Constitution and Composition of Cement Clinker

PII-24 SOPOUŠEK Jiri, FORET R.
Weld Joint Simulations of Heat-resistant Steels

PII-25 BURŠIK Jiří
Phase Equilibria in Ni-Al-Cr-Co-W-Re System: Modelling and Experiments

PII-26 KUZNETSOV V.N. and UDOVSKY Alexander L.
Comparing Stability Functions Derived from Experimental Thermodynamic Data and Calphad Calculations of the Co-Cr System as New Test of Assessments

PII-27 WNUK G., ROMANOWSKA Jolanta
Thermodynamic Properties of Liquid Sn-Zn-Cu Alloys

PII-28 ROMANOWSKA Jolanta, WNUK G.
Studies on Multicomponent Arsenic Systems

PII-29 BEŁTOWSKA-LEHMAN Ewa, OZGA P., ŚWIĄTEK Z., MICHALEC M. and LUPI C.
Non-equilibrium Phase Composition of Electrodeposited Zn-Ni Alloys

PII-30 OZGA Piotr
Equilibria in Aqueous Solutions of Ag(I)-Sn(II/IV) in Presence of Strong Complexing Ligands