

Oral Programme

Monday 28th May

Session 1

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| 8:30 - 9:00 | 1.1 | Plenary
TBA |
| 9:00 - 9:25 | 1.2 | First-principles calculation of a Fe-Pd phase diagram
<i>Tetsuo Mohri, Ying Chen & Takaharu Atago</i> |
| 9:25 - 9:50 | 1.3 | Modelling the Sigma-Phase Based on Equilibrium Volume First-Principles Calculations Results.
<i>Martin Friák, Mojmír Šob, Jana Houserová, Jan Vreštal</i> |
| 9:50 - 10:15 | 1.4 | Structural stability and electronic structure in trialuminides : ZrAl ₃ and HfAl ₃
<i>C. Colinet & A. Pasturel</i> |
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Coffee break

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|---------------|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:45 - 11:10 | 1.5 | Anomalous entropies of fusion
<i>Göran Grimvall</i> |
| 11:10 - 11:35 | 1.6 | Cluster Variation Method modelling of anti-phase boundary energies in multicomponent BCC alloys
<i>Cláudio Geraldo Schön & Ryoichi Kikuchi</i> |
| 11:35 - 12:00 | 1.7 | <i>Ab-initio</i> -Calphad prediction of the Mo-Ta-W phase diagram
<i>P.E.A. Turchi, Larry Kaufman & Zi-Kui Liu</i> |
| 12:00 - 12:25 | 1.8 | Estimation of thermodynamic properties of solutes in silicon
<i>Tooru Matsumiya, Keiji Iwata, Hideaki Sawada, Kazuto Kawakami & Tatsuo Ogasawara</i> |
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Lunch

Session 2

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|---------------|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00 - 14:25 | 2.1 | Computer simulation of the phase decomposition in superalloys based on the Phase Field Method in combination with the Cluster Variation Method
<i>Toshiyuki Koyama & Minoru Doi</i> |
| 14:25 - 14:50 | 2.2 | Computational Investigations on the Phase Decomposition Process in Multi-Components GaAsInP Alloy Systems based on the Phase Field Method
<i>Toru Miyazaki</i> |
| 14:50 - 15:15 | 2.3 | Molecular dynamics study of homogeneous nucleation of crystals in a supercooled liquid Pt with EAM potentials
<i>M. Jiang, K. Oikawa, C.C. Liew & T. Ikeshoji</i> |
| 15:15 - 15:40 | 2.4 | A Bayesian approach to evaluating the uncertainty of thermodynamic data and phase diagram
<i>Marius Stan & Brian Reardon</i> |
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Coffee break

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| 16:10 - 16:35 | 2.5 | Effect of interaction between chemical and magnetic ordering on the stability of Ni ₃ Fe (L1 ₂) ordered phase
<i>Ikuo Ohnuma, Yoshiyuki Himuro, Osamu Ikeda, Ryosuke Kainuma and Kiyohito Ishida</i> |
| 16:35 - 17:00 | 2.6 | Phase Equilibria between γ (A1) and γ' (L1 ₂) Phases in the Ni-rich Portion of the Fe-Ni-Si System
<i>Yoshiyuki Himuro, Ikuo Ohnuma, Ryosuke Kainuma and Kiyohito Ishida</i> |
| 17:00 - 17:25 | 2.7 | A Comparison of the Associate Model and the Random Solution Model of the Liquid Phase
<i>Koray Ozturk & Zi-Kui Liu</i> |
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Oral Programme

Tuesday 29th May

Session 3

- 8:30 - 9:00 3.1 Plenary
Arthur Pelton
- 9:00 - 9:25 3.2 MTDATA - Thermodynamic and Phase Equilibrium Software from the National Physical Laboratory
R.H. Davies, A.T. Dinsdale, J.A. Gisby, S.M. Martin and J.A.J. Robinson
- 9:25 - 9:50 3.3 Predicting phase equilibria in multicomponent oxide systems
J.A. Gisby, A.T. Dinsdale, J.R. Taylor & M.H. Rand
- 9:50 - 10:15 3.4 The information system on physico-chemical Properties of software package "Chemical Workbench"
G.V. Belov, M.A. Deminsky, V.S. Iorish and B.V. Potapkin
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Coffee break

- 10:45 - 11:10 3.5 PANDAT - A program for calculating thermodynamic multicomponent phase and related diagrams
Y. Austin Chang
- 11:10 - 11:35 3.6 Development of consistent multicomponent thermodynamic databases
Fan Zhang
- 11:35 - 12:00 3.7 Calculation of high order phase diagrams - 12 component Al-based system
Shuanglin Chen
- 12:00 - 12:25 3.8 Extending the thermodynamic magnesium alloy database
Rainer Schmid-Fetzer
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Lunch

Session 4

- 14:00 - 14:25 4.1 A computational tool for thermodynamical applications
Lars Höglund & Henrik Strandlund
- 14:25 - 14:50 4.2 Thermodynamic and diffusion calculations in multicomponent alloys - Examples of applications
Karin Frisk
- 14:50 - 15:15 4.3 Experimental and calculated carbon redistribution in steel weldments
Bořivoj Million, Jiří Sopoušek and Jan Vřešťál
- 15:15 - 15:40 4.4 Carburisation of iron: experiments and DICTRA simulations
A. Schneider, G. Inden & J. Zhang
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Coffee break

16:10 - 17:25

Poster Session

Presentation of FactSage

Oral Programme

Wednesday 30th May

Session 5

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| 8:30 - 9:00 | 5.1 | Plenary
Assessment of phases with internal degrees of freedom
<i>Bo Sundman</i> |
| 9:00 - 9:25 | 5.2 | Thermodynamic Modelling of C-Hf-Zr system
<i>H. Bittermann & P. Rogl</i> |
| 9:25 - 9:50 | 5.3 | Modelling glass transition and second order phase transformations
<i>G. Shao & Y.Q. Liu</i> |
| 9:50 - 10:15 | 5.4 | Thermodynamic modelling of the HDDR process in Sm-Fe alloys
<i>M. Zinkevich, N. Mattern & O. Gutfleisch</i> |
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Coffee break

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|---------------|-----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:45 - 11:10 | 5.5 | Application of thermodynamic modelling to the study of precipitation in IF (interstitial free) steels
<i>Roberto Avillez, André Costa e Silva & Fernando Rizzo</i> |
| 11:10 - 11:35 | 5.6 | Numerical simulation of phase decomposition in Fe-Cr binary and Fe-Cr-Mo ternary alloys with use of the Cahn-Hilliard equation
<i>Yoshihiro Suwa, Minoru Honjo & Yoshiyuki Saito</i> |
| 11:35 - 12:00 | 5.7 | On the stability of (Nb,Ti)(C,N) carbonitrides
<i>Byeong-Joo Lee</i> |
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12:00 - 13:00

Lunch

13:00 - 17:30

Conference excursion to Castle Howard

19:30

Conference banquet at St. William's College

Oral Programme

Thursday 31st May

Session 6

- 8:30 - 9:00 6.1 Plenary
Calphad thermodynamics
Larry Kaufman
- 9:00 - 9:25 6.2 Thermodynamics-aided alloy design of Pb-free solder system for high temperature applications
Jong Hoon Kim & Hyuck Mo Lee
- 9:25 - 9:50 6.3 Crystallography and phase equilibria
J.F. Smith
- 9:50 - 10:15 6.4 The prediction of mercury vapour pressures above amalgams for use in fluorescent lamps
A.T. Dinsdale, G.M. Forsdyke & S.A. Mucklejohn
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Coffee break

- 10:45 - 11:15 6.5 Influence of additives on the slag resistance of Al₂O₃-SiO₂-SiC-C bond phases under oxidising atmospheres
Chen-Feng Chan, Bernard B. Argent & William E. Lee
- 11:10 - 11:35 6.6 Prediction of the distribution of trace elements between the product streams of gasifiers, combustors and incinerators
Dennis Thompson, Bernard B. Argent & John H. Sharp
- 11:35 - 12:00 6.7 The O-U binary system : experimental state of the art and thermodynamic modelling
P.-Y Chevalier, E. Fischer and B. Cheynet
- 12:00 - 12:25 6.8 Thermodynamic modelling of oxide solid solutions and melt processing of Bi-2212 superconductors
Bengt Hallstedt & Ludwig J. Gauckler
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Lunch

Session 7

- 14:00 - 14:25 7.1 Thermodynamic assessment of the Si-B-C system
H.J. Seifert, B. Kasper, H.L. Lukas & F. Aldinger
- 14:25 - 14:50 7.2 Thermodynamic functions and phase diagram calculation for the Si₃N₄-Y₂O₃-SiO₂ system
O.B. Fabrichnaya, T. Ludwig, H.J. Seifert, F. Aldinger & A. Navrotsky
- 14:50 - 15:15 7.3 Thermodynamic optimisation and selected experiments in the systems Al-Mg-RE [RE = Sc, Ce, Gd, Y]
J. Gröbner, D. Kevorkov & R. Schmid-Fetzer
- 15:15 - 15:40 7.4 Discussion on the stability of the antimony-zinc binary phases
Marie-Christine Record, Véronique Izard, Jean-Claude Tedenac & Suzana G. Fries
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Coffee break

- 16:10 - 17:25 **Poster session**
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Oral Programme

Friday 1st June

Session 8

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| 8:30 - 9:00 | 8.1 | Plenary
"A garden of roses"
<i>Alan Oates</i> |
| 9:00 - 9:25 | 8.2 | Three-phase coexistence field (A ₂ +B ₂ +D ₀₃) and
phase decomposition in quaternary Fe-Al-Co-Ti alloys
<i>T. Kozakai, H. Araki, T. Koyama and M. Doi</i> |
| 9:25 - 9:50 | 8.3 | Estimation of viscosities of metallic and ionic melts from Gibbs energies of mixing
<i>R.E. Aune, Du Sichen & S. Seetharaman</i> |
| 9:50 - 10:15 | 8.4 | Theoretical and experimental study of the γ & γ' equilibrium in Ni-Al-Cr-Co and Ni-Al-Cr-W
systems
<i>P. Brož, J. Buršík, R. Picha and A. Kroupa</i> |

Coffee break

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| 10:45 - 11:05 | 8.5 | The prediction of thermophysical properties of high temperature metallic liquids
<i>J.A.J. Robinson, A.T. Dinsdale, L.A. Chapman & P.N. Quested</i> |
| 11:05 - 11:25 | 8.6 | Phase equilibria in the cobalt oxide - copper oxide system
<i>Leszek A. Zabdyr & Olga B. Fabrichnaya</i> |
| 11:25 - 11:45 | 8.7 | Partial and integral enthalpies of mixing of liquid Ag-Al-Cu and Ag-Cu-Zn alloys
<i>Victor T. Witusiewicz, Ulrike Hecht, Stephan Rex & Ferdinand Sommer</i> |
| 11:45 - 12:05 | 8.8 | Determination of the free energies of formation of Na ₂ Cr ₂ O ₄ and Na ₂ CrO ₄ using Na - β -Al ₂ O ₃ solid
electrolyte
<i>Vilas D. Tathavadkar & Animesh Jha</i> |
| 12:05 - 12:25 | 8.9 | A Thermodynamic Study of the Fe-Pt System
<i>P. Fredriksson, S. Seetharaman and B. Sundman</i> |

Lunch

End of conference
