



**TOFA 2012 – DISCUSSION MEETING  
ON THERMODYNAMICS OF ALLOYS  
September 23 – 28, 2012 • Pula, Croatia**



**SUNDAY 23 September, 2012**

**Conference Venue and Registration**

**16:00 – 19:00 Registration desk open (Hotel HISTRIA outside the meeting room)**

**19:30 Welcome Drink**

**20:00 Welcome Dinner**

**MONDAY 24 September, 2012**

**08:30 – 09:00 Registration desk open (Hotel HISTRIA outside the meeting room)**

**09:00 – 09:30 Welcome**

**09:30 – 10:10 PL1 Richter K., Vienna University - Austria**  
Partial ordering in structurally complex solid solution phases

**10:10 – 10:30 O1 Colinet C., Tedenac J.-C.**  
A first principles study of point defects and site occupancy in  $D8_m\text{-Nb}_5\text{Si}_3$ ,  $D8_l\text{-Nb}_5\text{Si}_3$ ,  $D8_m\text{-Mo}_5\text{Si}_3$

**10:30 – 10:50 O2 Ishida K.**  
Phase equilibria and phase transformations in Fe-Mn based alloys

**10:50 – 11:20 Coffee break**

**11:20 – 11:40 O3 Zeiringer I., Grytsiv A., Koblyuk N., Brož P., Rogl P.**  
Phase relations and melting behaviour in clathrate systems  $\text{Ba}_8\{\text{Cu,Ag,Au}\}_x\{\text{Si,Ge}\}_{46-x}$

**11:40 – 12:00 O4 Mohri T., Kiyokane N., Chen Y.**  
Applications of CDCVM to the study of alloy phase equilibria

**12:00 – 12:20 O5 Yin M., Nash P., Du Y.**  
Enthalpies of formation and specific heat of selected Heusler alloys  $\text{Ni}_2\text{XY}$  (X=Zr, Hf, V, Nb, Ta, Mn; Y=Al, In, Si, Sn)

**12:20 – 12:40 O6 Ohnuma I., Shimenouchi S., Omori T., Kainuma R., Ishida K.**  
Experimental investigation of phase equilibria at low temperatures ( $< 600^\circ\text{C}$ ) in the Fe-Ni binary system

**12:40-15:00 Lunch**

**15:00 – 15:30 KN1 Joubert J.-M., CNRS-Université Paris Est, France**  
Phase diagram of Fe-Ti-V system and related hydrogen storage properties

- 15:30 – 15:50 O7 Krendelsberger N., Stein F., Weitzer F., Schuster J.C.**  
Phase equilibria of the partial system  $\text{CoSiTi} - \text{Ti}_5\text{Si}_3 - \text{TiSi} - \text{Co}_4\text{Si}_7\text{Ti}_4$
- 15:50 – 16:10 O8 Schmitz S., Löser W., Lindenkreuz H.G., Büchner B.**  
Liquid phase separation, solidification and phase transformations of Gd-Ti and Gd-Ti-Al-Cu alloys
- 16:10 – 16:30 O9 Witusiewicz V.T., Bondar A.A., Hecht U., Sleptsov S.V., Hallstedt B.**  
Experimental study and thermodynamic remodelling of the ternary Ti-Al-C system

**16:30 – 17:00 Coffee break**

- 17:00 – 17:30 KN2 Fries S., ICAMS, Ruhr-Universität Bochum, Germany**  
Theory and experiments: opponents in a close alliance

- 17:30 – 17:50 O10 Skolyszewska-Kühberger B., Ganesan R., Ghosh S., Ipser H.**  
Interaction of rare earth elements with Cd: thermochemistry and phase equilibria in the systems Cd-Nd and Cd-Ce
- 17:50 – 18:10 O11 Chen Y., Hirosawa S., Iwata S.**  
First principles modeling of formation and stability of fcc- $\text{NdO}_x$  at Nd / Nd-Fe-B interface.
- 18:10 – 18:30 O12 Mattern N.**  
Experimental and thermodynamic assessment of the Gd-Zr and Gd-Ti phase diagrams
- 18:30 – 18:50 O13 Medved J., Volšak D., Vončina M., Markoli B., Mrvar P.**  
Thermodynamic characterization of aluminium corner of Al-Cu-Nd

## **TUESDAY 25 September, 2012**

- 08:30 – 09:10 PL2 Chatain D., CNRS, Aix-Marseille University, France**  
Compositional transitions at surfaces and grain boundaries vs. bulk phase transitions
- 09:10 – 09:30 O14 Artini C., Muolo M.L., Passerone A., Valenza F., Cacciamani G.**  
Wettability and interfacial reactions in the (Ni,B)/ $\text{ZrB}_2$  system
- 09:30 – 09:50 O15 Vingurt D., Fuks D., Landau M.**  
Grain boundaries on the surface of MgO as a precursor for improved catalytic activity: DFT study
- 09:50 – 10:10 O16 Eiken J., Apel M.**  
Phase-field simulations of the solidification of hypoeutectic Al-Si cast alloy based on thermodynamic and chemical mobility databases
- 10:10 – 10:30 O17 Schmachtel S., Taskinen P.**  
Critical thermodynamic evaluation of the Pb-Sb system including equilibration tests to determine solid solubilities of lead in antimony and vice versa

**10:30 – 11:30 Coffee break and Poster Session**

- 11:30 – 12:00 KN3 Plevachuk Y., Ivan Franko National University, Lviv, Ukraine**  
Thermophysical properties and microsegregation of liquid metal eutectic alloys
- 12:00 – 12:20 O18 Yakymovych A., Elmahfoudi A., Sklyarchuk V., Plevachuk Yu., Flandorfer H., Ipser H.**  
Electrical conductivity and enthalpy of mixing of Co-Sn liquid alloys

**12:20-15:00 Lunch**

**15:00 – 15:30**      **KN4**   **Cacciamani G., Genoa University, Italy**  
Experimental investigation and thermodynamic modelling of the Co-Ni-Ti system

**15:30 – 15:50**      **O19**   **Bittner R., Duarte L., Leinenbach C., Richter K. W.**  
Phase diagram of aluminum-germanium-titanium.

**15:50 – 16:10**      **O20**   **Eleno L.T.F., Gonzales-Ormeño P.G., Petrilli H.M., Schön C.G.**  
Ordering phase relations in ternary iron aluminides

**16:10 – 16:30**      **O21**   **Zemanova A., Schmetterer C., Kroupa A., Rajamohan D., Flandorfer H.**

The experimental and theoretical study of the In-Ni-Sn system

**16:30 – 16:50**      **O22**   **Jendrzeczyk-Handzlik D., Fitzner K.**  
Thermodynamic properties of the ternary liquid Ag-Cu-Ga system

**16:50 – 17:50 Coffee break and Poster Session**

**17:50 – 18:10**      **O23**   **Meschel S.V., Nash P., Gao Q.N., Wang J.C., Du Y.**  
The standard enthalpies of formation of some binary intermetallic compounds of lanthanide – iron systems by high temperature direct synthesis calorimetry

**18:10 – 18:30**      **O24**   **Klancnik G., Medved M.**  
Phase transformations and thermodynamic description of Al-Sb-Zn alloys

**WEDNESDAY 26 September, 2012**

**08:30 – 09:10**      **PL3**   **Meyer A., Institute of Materials Physics in Space, German Aerospace Center (DLR), Cologne, Germany**  
Diffusion of mass in liquid metals and alloys

**09:10 – 09:30**      **O25**   **Amore S., Nowak R., Bruzda G., Korpala B., Sobczak N., Tuissi A., Giuranno D., Novakovic R., Ricci E.**  
Thermodynamics and surface properties of liquid Si-Ge alloys

**09:30 – 09:50**      **O26**   **Brillo J., Schick M., Schmitz J., Egry I.**  
Density and viscosity of liquid Al-Cu-Si alloys

**09:50 – 10:10**      **O27**   **Urrutia A., Tumminello S., Sommadossi S.**  
Novel growing intermediate phases in Ni/Al diffusion-reaction couples

**10:10 – 10:30**      **O28**   **Dalla Fontana G., Fiore G.L., Battezzati L.**  
Thermodynamics of a Au-based glass-forming alloy

**10:30 – 11:00 Coffee break and Poster Session**

**11:00 – 11:20**      **O29**   **Rogl P.F., Tanaka T., Takenouchi S., Vrestal J.**  
Peritectic melting of  $\beta$ -boron in B-C binary

**11:20 – 11:40**      **O30**   **Lacaze J., Jackson K.A.**  
Experimental study and simulation of reverse spinodal decomposition

**11:40 – 12:00**      **O31**   **Watson A.**  
The use of PANDAT software in thermodynamic calculations relating to lead-free solder alloys

**12:00 – 13:00 Lunch**

**13:00 Excursion to Brionian Islands**

**20:00 Conference Dinner**

## **THURSDAY 27 September, 2012**

**09:00 – 09:40 PL4 Marks L.D., Department of Materials Science and Engineering, Northwestern University, USA**

Nanoparticles: from Wulff to Winterbottom, Plasmonics, Catalysis and Nanoalloys

**09:40 – 10:00 O32 Park J.H., Paik D.J.**

Thermodynamics of the formation of Zn-Al-Fe intermetallic compounds in molten zinc bath

**10:00 – 10:20 O33 Shimenouchi S., Ohnuma I., Omori T., Ishida K., Kainuma R.**

Coherent and incoherent phase equilibria of bcc miscibility gap in the Fe-Al system

**10:20 – 10:40 O34 Coelho G.C., da Silva A.A.A.P., Nunes C.A., Suzuki P.A.**

Experimental study of the Ta-Ge system

### **10:40 – 11:10 Coffee break**

**11:10 – 11:40 KN5 J. Lee, Korea University, Seoul, Korea**

Thermochemistry measurements from electrostatic levitation experiments

**11:40 – 12:00 O35 Mouas M., Gasser J.-G., Hellal S.**

Structure and dynamics in liquid solders: structure factor, diffusion coefficients, viscosity and isothermal compressibility

**12:00 – 12:20 O36 Lapsa J., Onderka B.**

Thermodynamic properties of liquid Ag-Sb-Sn alloys determined from e.m.f. and calorimetric measurements

**12:20 – 12:40 O37 Nunes C.A., Fiorani J.M., Ferreira F., David N., Coelho G.C., Vilasi M.**

Thermodynamic optimization of the V-Si-B system

### **12:40 – 15:00 Lunch**

**15:00 – 15:20 O38 Du Y., Wang P., Liu L., Bo H., Xu H., Wang M., Liu S., Chen H.-L., Chen Q., Engström A.**

Experimental investigation and thermodynamic modeling of the multicomponent Mg alloys

**15:20 – 15:40 O39 Utton C.A., Xu Z., Papadimitriou I., Kinoshita H., Tsakiroopoulos P.**

Phase equilibria in niobium silicide-based alloys

**15:40 – 16:00 O40 Khvan A.V., Hallstedt B., Chang K.**

Thermodynamic assessment of Cr-Nb-C and Mn-Nb-C systems

**16:00 – 16:20 O41 Stifanese R., Delsante S., Borzone G.**

Experimental investigation of the R-Ni (R= rare earth) systems: enthalpy of formation of the RNi<sub>2</sub> phases.

**16:20 – 16:40 O42 Chatain S., Alpettaz T., Gueneau C., Gosse S., Chatillon C., Dupin N.**

Thermodynamic study of uranium – silicon – carbon system: silicon activity measurements and thermodynamic modelling

**16:40 – 17:00 O43 Fabrichnaya O., Savinykh G., Schreiber G.**

Phase relations in the ZrO<sub>2</sub>-La<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> system: experimental investigation and thermodynamic modelling

**17:00 – 19:00 Nanoalloys Workshop COST MP0903**

**Poster Session & Coffee Break**

## **FRIDAY 28 September, 2012**

### **Nanoalloys Workshop COST MP0903**

**08:30 – 08:40**            **Ferrando R., Genoa University, Italy**  
**The COST Action MP0903**

**08:40 – 09:20**            **PL5 Johnston R.L., University of Birmingham, UK**  
Simulating the structures and chemical ordering of nanoalloys

**09:20 – 09:40**            **O44 Kaptay G.**  
The nano-CALPHAD concept

**09:40 – 10:00**            **O45 Lee J.**  
Phase stability of small metallic particles: experiments and CALPHAD theories

**10:00 – 10:20**            **O46 Vrestal J., Pinkas J., Sopoušek J., Brož P.**  
Thermodynamic calculation of phase diagrams of nanoalloys

**10:20 – 10:40**            **O47 Mottet C., Biancarelli-Lopes A., Tréglia G.**  
Bimetallic nanoparticle modeling: towards nanoalloys phase diagrams

### **10.40 – 11.10 Coffee break**

**11:10 – 11:40**            **KN6 Baletto F., Physics Department, King's College London, UK**  
Energetic, thermodynamics and kinetics of metallic nanoalloys

**11:40 – 12:00**            **O48 Polak M., Rubinovich L.**  
Thermodynamical aspects of phase separation transitions in binary and ternary nanoalloys

**12:00 – 12:20**            **O49 Hou M.**  
Relationships between alloy and nanoalloy phase diagrams – an atomistic view

**12:20 Concluding Remarks**