THERMODYNAMICS OF ALLOYS
SEPTEMBER 23-28, 2012
PULA

TOFA 2012

DISCUSSION MEETING ON THERMODYNAMICS OF ALLOYS

Selected peer reviewed abstracts and programme of
TOFA 2012 - Discussion Meeting on Thermodynamics of Alloys

September 23 – 28, 2012
Pula, Croatia

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TOFA 2012

Programme

of the

Discussion Meeting on THERMODYNAMICS OF ALLOYS

September 23 – 28, 2012
Hotel Histria Park, Pula, Croatia

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
Chairs: Borzone G., Ipser H.
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 $D8_m$-Nb_5Si_3, $D8_l$-Nb_5Si_3, $D8_m$-Mo_5Si_3
10:30 – 10:50 O2 Ishida K.
Phase equilibria and phase transformations in Fe-Mn based alloys

10:50 – 11:20 Coffee break

Chairs: Meschel S.V., Kroupa A.
11:20 – 11:40 O3 Zeiringer I., Grytsiv A., Koblyuk N., Brož P., Rogl P.
Phase relations and melting behaviour in clathrate systems $Ba_8\{Cu,Ag,Au\}_x\{Si,Ge\}_{46-x}$
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 Ni_2XY (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°C) in the Fe-Ni binary system

12:40-15:00 Lunch

Chairs: Ishida K., Du Y.
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 CoSiTi – Ti_5Si_3 – TiSi – $Co_4Si_7Ti_4$
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

Chairs: Delsante S., Nash P.
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-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

Chairs: Novakovic R., Lee J.
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)/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

Chairs: Vrestal J., Brillo J.
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

Chairs: Sommadossi S., Rogl P.
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 Jendrzejczyk-Handzlik D., Fitzner K.
Thermodynamic properties of the ternary liquid Ag-Cu-Ga system

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

Chairs: Zivkovic D., Schuster J.
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

Chairs: Ricci E., Schön C.G.
08:30 – 09:10 PL3 Meyer A., Institute of Materials Physiscs 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

Chairs: Colinet C., Mohri A.
11:00 – 11:20 O29 Rogl P.F., Tanaka T., Takenouchi S., Vrestal J.
Peritectic melting of ß-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

Chairs: Watson A., Fiorani J.-M.
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

Chairs: Janczak-Rusch J., Fitzner K.
11:10 – 11:40 KN5 Lee J., 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 Łapsa 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

Chairs: Fries G.S., Mikula A.
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.,Tsakiropoulos 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$_2$ 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$_2$-La$_2$O$_3$-Y$_2$O$_3$-Al$_2$O$_3$ 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
Chairs:Ferrando R.
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

Chairs: Mottet C.

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

POSTER PRESENTATIONS

P1 Allam A., Boulet P., Nunes C.A., Record M.C.
Experimental investigations of the stability of the higher manganese silicides

P2 Belov A.N., Bulyarsky S.V., Gromov D.G., Pavlova L.M., Pyatilova O.V.
Study of silver cluster formation from thin films on inert surface

P3 Cacciamani G., Muolo M.L., Passerone A., Valenza F., Artini C.
Thermodynamic study of the ternary B-Ni-X systems (X ≡ Ti, Zr, Hf)

P4 Chaia N., David N., Fiorani J.M., Mathieu S., Coelho G.C., Nunes C.A., Vilasi M.
The assessment of phase equilibria in V-Cr-Si system

P5 Colinet C., Tedenac J.-C.
Stability of ternary compounds with the Fe_2P-type structure

P6 da Silva A.A.A.P., Fiorani J.M., Coelho G.C., Nunes C.A., David N., Vilasi M.
Thermodynamic modelling of the Fe-Nb system

P7 Dêbski A., Gąsior W.
ENTALL - thermodynamics database of alloys for safe hydrogen storage and energy

P8 Delsante S., Borzone G.
Calorimetric investigation of rare earth-magnesium alloys

P9 Eleno L.T.F., Petrilli H.M., Schön C.G.
A preliminary assessment of the Nb – Ni – Si system using ab-initio data

P10 Falmbigl M., Grytsiv A., Rogl P., Kneidinger F., Bauer E., Effenberger H.
Crystal structures, phase relations, physical properties and DFT calculations in the Ge-rich part of the Ba-Rh-Ge system

P11 Fima P., Garzeł G.
Thermal analysis of the Ag-Bi-Cu system

P12 Gąsior W.
Modeling of viscosity of binary alloys for SURDAT-database. comparative study

P13 Giuranno D., Ricci E., Arato E.
Modelling of oxygen transport applied to the Si-Ge system

P14 Gossé S., Guéneau C., Brackx E., Dugne O., Chatain S.
Thermodynamic study of the Nickel-Palladium-Tellurium system

P15 Jandl I., Reichmann T.L., Richter K.W.
The Al-Ge-Ni phase diagram

P16 Kaban I., Mattern N., Eckert J.
Thermophysical properties and wetting behaviour of SnSb-based alloys

P17 Kaptay G.
The 4th law of thermodynamics

P18 Kish O., Froumin N., Salhov S., Barzilai S., Gelbstein M., Aizenshtein M., Frage N.
Interface interaction and wetting in the Ta_2O_5/Cu-Me (Me=Al, Ti) systems

P19 Koltsov V.B., Mikhailova M.S.
The electronic part of melting entropy and electronic states spectrum in semiconductor melts

P20 Koltsov V.B., Mikhailova M.S.
About change of effective mass of states' density and electrons mobility at the melting of metalizing semiconductors

P21 Lussana D., Baldissin D., Lombardo D., Miranti L., Castellero A., Rizzi P., Balducci E., Massazza M., Baricco M.
Thermodynamic aspects of high temperature oxidation on a 304 stainless steel

P22 Manasijević D., Živković D., Talijan N., Ćosović V., Gomidželović L., Todorović R., Minić D.
Experimental investigation and thermodynamic calculation of the Au–Ga–Sb phase diagram

P23 Mekler C., Vegh A., Kaptay G.
Bulk and surface thermodynamics of monotectic liquid alloys

P24 Minić D., Manasijević D., Ćosović V., Živković D., Talijan N., Premović M.
Phase transformations in the ternary Ag–Ga–Sb system

P25 Montanari R., Varone A.,
Transformations in liquid hypo- and eutectic Pb-Bi alloys

P26 Nyk J., Onderka B.
Interaction of oxygen in ternary liquid Ag-X-O alloys

P27 Oudich F., David N., Fiorani J.M., Vilasi M.
Contribution to the thermodynamic description of the Bi_2O_3-Al_2O_3-PbO system

P28 Pavlova L.M., Prokofieva V.K.
The relationship between the phase diagram, structure and thermodynamic properties in the Ba – Ge system

P29 Pavlu J., Vreštal J., Štrof J., Wdowik U.D., Šob M., Buršik J.
Stability of Laves phase in the V-Zr system below room temperature

P30 Plevachuk Yu., Sklyarchuk V., Eckert S., Gerbeth G., Novakovic R.
Thermophysical properties of liquid Ga-In-Sn eutectic alloy

P31 Rajamohan D., Schmetterer C., Flandorfer H., Ipser H.,
High temperature lead-free soldering: phase equilibria of (Cu, Ni)-Sn-Zn system

P32 Ritscher A., Richter K.W., Kroupa A., Ipser H.,
Pressure dependence of the phase equilibria in the Sn-P system

P33 Romanowska J.
Numerical prediction of thermodynamic properties of ternary alloys

P34 Romanowska J.
Aluminium diffusion in aluminide coatings deposited by the CVD method on pure Nickel

P35 Romanowska J.
Calorimetric study of some Bi-Cu-Sn alloys

P36 Sufryd K., Riani P., Cacciamani G.
The Co-Ni-Ti isothermal section at 900 °C

P37 Trybula M., Gasior W.
Thermodynamic and physical properties of liquid alloy in terms of free volume theory

P38 Voncina M., Medved J.
Impact of Ce addition on Cu phases in A380 alloy

P39 Wind J., Romaniv O., Schöllhammer G., Bursik J., Giester G., Rogl P.,
The systems Tantalum (Niobium) – Cobalt – Boron

P40 Yuan Y., Watson A., Li D., Pan F., Tang A.
An assessment of the Mg-Fe-Si system

P41 Živković D., Balanović Lj., Gomidželović L., Manasijević D., Talijan N., Kostov A., Ćosović V., Minić D.
Thermodynamics and phase equilibria of Ga-Me (Me = Al, Au) alloys

WORKSHOP COSTMP0903

P42 Atanasov I., Sloan C., Ahmed M., Warnken N., Ferrando R., Johnston R.L.
Size dependance of the chemical ordering of Cu-Ag nanoparticles

P43 Bochicchio D., Ferrando R.
Structure and thermodynamics of Ag-Cu nanoalloys: a computational study

P44 Delsante S., Borzone G., Pigozzi G., Janczak-Rusch J.
Metal nanoparticles: synthesis, morphology and thermal behaviour

P45 Janczak-Rusch J., Garzel G., Zabdyr L.
The effect of the phase size and shape on the Ag-Cu (nano) phase diagram

P46 Kroupa A., Kana T., Sob M.
The calculation of the phase diagrams of nanoalloys using *ab-initio* surface tension calculations

P47 Mishra R., Zemanova A., Kroupa A., Flandorfer H., Ipser H.
Synthesis and characterization of Sn-rich Ni–Sb–Sn nanosolders

P48 Novakovic R., Calvò F, Ferrando R.
About the modelling of the surface tension of liquid Ag-Au alloys

P49 Pignedoli C.A., Gaspari R., Prinz J., Vogt J., Gille P., Armbrüster M., Brune H., Gröning O., Passerone D., Widmer R.
Unravelling the surface structure of PdGa intermetallic compound by *ab initio* thermodynamics

P50 Watson A., Novakovic R.
Extension of thermodynamic database for the calculation of nano-sized phase diagrams

ORAL PRESENTATIONS

PL1

PARTIAL ORDERING IN STRUCTURALLY COMPLEX SOLID SOLUTION PHASES

K.W. Richter

Department of Inorganic Chemistry - Materials Chemistry, University of Vienna, Austria

The correct modelling of homogeneity ranges in solid solutions is a major challenge in CALPHAD-type thermodynamic phase diagram assessment. Crystallographic information on defect mechanisms has to be employed to construct correct models suitable for extrapolation into higher order systems. While much work has been done to address this problem for the most important simple intermetallic crystal structures, the solid solution formation for higher order intermetallics with complex crystal structure is not well investigated up to now. In a recent research project we performed an extended case study on substitution and partial ordering in several ternary systems combining two early transition metals (M, M' = V, Nb, Ta, Zr, Hf) with As, Ge and Ga. Solid solution phases and ternary compounds observed in these systems usually show considerable substitution among the two (chemically closely related) transition metals M and M'. However, M and M' are never distributed randomly over all available metal sites, but rather show strong preferences to specific sites. Preferred site occupation is even found for the pair Zr / Hf which is considered to be the most closely related pair of homologous elements in the periodic system.

Site preferences can usually be rationalized by structural arguments and bonding considerations. For the modelling of site occupations we used ground state energies of (hypothetical) isostructural ordered compounds (End members) which were obtained from ab-initio DFT calculations. By implementing these values to the well-known Compound Energy Formalism (CEF) used in CALPHAD modelling, we could predict the experimentally observed site preferences with good accuracy. In case of closely related structures it was furthermore possible to predict the relative stability of the partially ordered compounds at elevated temperatures without any excess term to the modelled Gibbs energy. Consequences of our results for thermodynamic modelling as well as for exploratory synthesis purposes will be discussed.

PL2

COMPOSITIONAL TRANSITIONS AT SURFACES AND GRAIN BOUNDARIES VS. BULK PHASE TRANSITIONS

D. Chatain [1], P. Wynblatt [2]

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[2] *Department of Materials Science and Engineering, Carnegie Mellon University,*
Pittsburgh PA 15213, USA

This presentation aims to describe the similarities and differences between the phase transitions which occur in bulk multicomponent systems, and the compositional transitions that may occur at surfaces and interfaces.

Compositional transitions at interfaces in multi-component systems can result in the formation of adsorbed layers of widely varying thickness, from less than one atomic monolayer to several tens of monolayer. In cases where the adsorbed layers are relatively thick they have often been referred to in the literature as surficial films, complexions or wetting layers, and may be confused with bulk phases. The origin of these adsorbed layers is closely associated with the presence of wetting transitions, which are interfacial phenomena taking place between bulk phases.

This paper will provide an overview of the effects of composition and temperature on surface/interface layer thickness, obtained by modeling adsorption at surfaces and grain boundaries. Relevant experimental observations of compositional transitions at the surfaces of several metallic alloy systems will also be summarized.

PL3

DIFFUSION OF MASS IN LIQUID METALS AND ALLOYS

A. Meyer

Institute of Materials Physics in Space, German Aerospace Center, 51170 Cologne, Germany

Atomic diffusion is a fundamental property for an understanding of liquid dynamics, nucleation, vitrification, and crystal growth. Diffusion data serve as a vital input to the modeling of microstructure evolution and are an essential control to molecular dynamics simulation results. A common method to measure diffusion coefficient in liquid alloys is the long capillary (LC) technique and its variations. There, a diffusion couple of different composition, in the case of interdiffusion, or containing a different amount of isotopes, in the case of self diffusion, is annealed in the liquid state and subsequently quenched to ambient temperature. The diffusion profiles are analyzed post mortem. This technique exhibits several drawbacks that in most cases prevent an accurate measurement of diffusion coefficients - convective contributions during diffusion annealing are the most prominent ones.

Recently, the field of liquid diffusion experiments advanced through the use of quasielastic neutron scattering (QNS) on levitated metallic droplets for accurate measurements of self-diffusion coefficients in high temperature metallic liquids. For the accurate measurement of interdiffusion we combine LC experiments with an in situ monitoring of the entire interdiffusion process by the use of X-ray and neutron radiography. These experiments are accompanied by diffusion experiments in space in order to benefit from the purely diffusive transport under microgravity conditions for a large variety of alloy systems.

In this presentation recent experimental results are discussed in the context of the relation of self- and interdiffusion (Darken’s equation), of the relation of self diffusion and viscosity (Stokes-Einstein relation), as well as of the importance of accurate transport coefficients for the modeling of crystal growth.

PL4

NANOPARTICLES: FROM WULFF TO WINTERBOTTOM, PLASMONICS, CATALYSIS AND NANOALLOYS

D. Alpay, S. Patala, L. Peng, E. Ringe, L.D. Marks

Department of Materials Science and Engineering, Northwestern University,
Evanston, IL 60208

Understanding the structure of nanoparticles is a problem with over a century of history from the first analysis by Wulff[1] which was only proved during WWII by von Laue[2], the extension for supported particles on a flat substrate by Winterbottom[3] _ENREF_8 and at an edge by Taylor et al[4]. All these analyses have focused on single crystals, but often nanoparticles have different structures as first shown by of Ino and Ogawa[5-7] who published just ahead of Allpress and Sanders[8]. These structures, called multiply-twinned particles or MTPs remained incompletely understood until a variant of a Wulff construction was shown to explain their equilibrium shapes[9-11]. Given the growth of nanotechnology in the last decades, significant advances in synthesis and characterization methods have been made so it is time to return to some of these topics and look further. It appears there is still a fair amount of science left to be done, ranging from Wulff shapes for alloys[12] to understanding the growth shapes of nanoparticles based upon a kinetic variant of the modified Wulff construction[13]. Some recent results such as finite size effects for alloys and single-phase nanoparticles and how this couples with the chemical potential and substrate interfacial energy, as well as how these relate to applied topics such as nanoplasmonics and face-selective catalysis will be described. _ENREF_21

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[2] M. von Laue, Z. Kristallogr., 105 (1943) 124.
[3] W. L. Winterbottom, Acta Metal., 15 (1967) 303.
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SIMULATING THE STRUCTURES AND CHEMICAL ORDERING OF NANOALLOYS

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Keywords: Melting; Nanoalloys; Segregation; Simulation; Thermodynamics

Nanoalloys (bi- and multimetallic nanoparticles) are the subject of considerable interest due to their potential application in fields ranging from catalysis (including fuel cell electrocatalysis) to electronics, optics (including plasmonics), magnetics and sensor technology (including biosensors)[1,2]. It is known that the chemical and physical properties of nanoalloys depend critically on their size, morphology, composition and chemical ordering, so it is important to know how these can be controlled during their synthesis or by processing. Also of interest is how nanoalloy structures are influenced by their environment: what is the effect of surfactant molecules, gaseous adsorbates, solvent or supporting substrate? Comparisons with bulk bimetallic systems are also of interest, with the development of nanoalloy "phase diagrams" (which depend on size as well as temperature and composition) being a particular challenge.

In this presentation, I will start with a brief overview of the field of nanoalloys and of theoretical techniques used to study their structures, chemical ordering and phase behaviour. This will be followed by examples from our research into: the global optimisation of nanoalloy structure and chemical ordering[3,4]; studies of melting of nanoalloys[5]; and simulations of size-dependent changes in elemental segregation of copper-silver nanoparticles[6]. Comparisons will be made with experiments, where available.

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KN1

PHASE DIAGRAM OF Fe-Ti-V SYSTEM AND RELATED HYDROGEN STORAGE PROPERTIES

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Keywords: Hydrogen storage; bcc solid solutions; Ti-V-Fe; Phase diagram

Light vanadium-based alloys crystallizing in the body centered cubic (bcc) structure are promising materials for hydrogen storage. Adding titanium to vanadium improves the kinetics of the hydrogen absorption whereas addition of 3d metals such as iron enhances the reversible absorption capacity and the activation process. The aim of this study is to highlight the influence of alloy composition on the hydrogenation properties (absorption pressure and capacity) of the bcc phase. The isothermal sections at 1000°C and 1200°C of the Fe-Ti-V system have been studied experimentally[1] to gain a better knowledge of the bcc-region boundaries and the nature of the equilibrium phases. Alloys have then been synthesized in both single bcc phase region and with various amounts of precipitated phases. The hydrogen pressure-composition isotherms of these alloys have finally been characterized at different temperatures demonstrating the influence of the composition and the microstructure on the hydrogen storage properties[2, 3].

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KN2

THEORY AND EXPERIMENTS: OPPONENTS IN A CLOSE ALLIANCE

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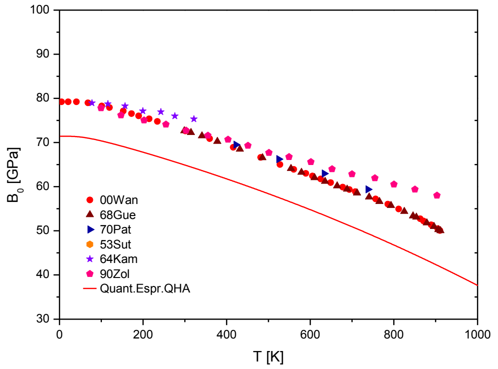
Aristotle's approach to the understanding of nature did not include experiments. In his model women were supposed to have less teeth than men. It took sometime till the experiment was done demonstrating that his prediction was incorrect.

During the last century many experiments were done which discover and determine materials behaviour, however, only since the last years a quantum mechanical theoretical approach was developed and implemented that could, in a way, predicts some of the experimental facts related to phase stability. This success implied in a increased confidence on theoretical methods, with a subsequent detriment of experiments.

Now-a-days when many quantum mechanics theoretical predictions for materials properties as volumes, enthalpies of formation, heat capacity, bulk modules, elastic constants, etc.., it is shown that when one "is counting the teeth" some surprises can appears. The figure shows an example where the bulk modulus predicted by the density functional theory for Al in the fcc crystal structure is compared to experiments. That kind of results enhance the importance of experiments as the theoretical predictions must be validated.



The figure shows the bulk modulus of Aluminium calculated in the quasi-harmonic approximation compared to experimental data (unpublished work by Mauro Palumbo and co-workers)

In this lecture, several examples will be shown where experiments are required, which will result in the improvement of the theoretical development.

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KN3

THERMOPHYSICAL PROPERTIES AND MICROSEGREGATION OF LIQUID METAL EUTECTIC ALLOYS

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Keywords: Melting; Nanoalloys; Segregation; Simulation; Thermodynamics

Binary and ternary lead and tin-based eutectic metal alloys are constantly in focus of research as a basis for new advanced materials for industrial applications. Investigations of their eutectic regions have often revealed uncharacteristic behavior of some physical properties. Molten metallic alloys have been demonstrated to undergo a number of structural transformations from the initial microheterogeneous state immediately after melting to the true solution state.

The solidification process of a liquid alloy has a profound impact on the structure and properties of the solid material. Therefore, knowledge of the physical properties of the molten alloys prior to solidification becomes very important for the development of materials with predetermined characteristics.

The presented results of thermophysical properties (surface tension, density, electrical and thermal conductivity, viscosity) of eutectic systems with simple and complicated phase diagrams, obtained in a wide temperature interval above the liquidus including a melting-solidification range, revealed their anomalous behaviour well above the liquidus. The temperature range of anomalies reached hundreds of degrees. The obtained results are interpreted assuming that microsegregation areas exist in the eutectic melts. The ascertained inconsistencies have confirmed an existence of areas of different thermodynamic stabilities in the liquid state. These regions manifest themselves as anomalous fluctuations of the concentration, which is reflected, in turn, in a change of the generally foreseen physical properties. In this context, the influence of heat treatment of a molten metallic alloy on the structure and properties of the final material within a specific working temperature range becomes significant.

KN4

EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC MODELLING Of THE Co-Ni-Ti SYSTEM

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Co-Ni-Ti is an important ternary sub-system relevant to different kinds of applications: from Ni-based superalloys to hard magnetic materials, from Ti-based corrosion-resistant alloys to amorphous and metastable phases. Moreover, from a more fundamental point of view, it is an interesting example of a system where both structural and magnetic ordering occur and interact, especially when considered as a subsystem of the Co-Fe-Ni-Ti quaternary.

This system has been studied by several investigators using diffusion couples and equilibrated alloys. Several isothermal sections and a pseudobinary CoTi-NiTi section were established. The isothermal sections agree to each other in the Ti-richer part (at $x(\mathrm{Ti}) > 0.5$). However, at lower Ti content contradictory results appear, especially concerning the phases at the Ti(Co,Ni)3 ratio.

To solve such uncertainties a reinvestigation of the system has been carried out by both experiments and thermodynamic modelling.

Several samples have been prepared by arc melting, equilibrated at 900 °C and characterised by optical and electronic microscopy, electron probe microanalysis and X-ray diffraction. In this way the 900°C isothermal phase diagram has been determined.

The experimental investigation has been complemented by a thermodynamic modelling of the system and, in particular, of the ordering transformations occurring between the fcc- and bcc-based phases either in the stable or metastable states. For both fcc and bcc phases four sublattice models have been adopted and ordering phenomena have been explicitly accounted for. Moreover, a series of constraints and relations between the interaction parameters of structurally related phases have been introduced. As a result stable as well as metastable Co-Ni-Ti equilibria have been thoroughly described.

KN5

THERMOCHEMISTRY MEASUREMENTS FROM ELECTROSTATIC LEVITATION EXPERIMENTS

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Recently, electrostatic levitation technique gains lots of interests from thermochemistry researchers. Conventional methods for thermochemistry make use of a certain container, which may react with liquid metals or alloys in it at high temperatures. Therefore, in many cases, the conventional methods have many restrictions in measurements such as temperature range, atmosphere, containers, etc. For example, surface tension and density can be measured by using the sessile drop method. However, selection of substrate (or crucible) is limited to prevent any possible chemical reactions. Moreover, data of undercooled sample is impossible to obtain. On the other hand, levitation technique makes it possible to prevent any possible reactions, and enables measurements of undercooled samples. When we compare the electromagnetic levitation and the electrostatic levitation, the former has a merit to do experiments in controlled atmosphere, and the latter is useful to measure viscosity simultaneously. Recently, a new experimental system for electrostatic levitation and thermochemistry measurements has been made in KRISS, Korea. In this presentation, we report our new experimental data and possible applications such as nano phase diagram.

KN6-COSTMP0903

ENERGETIC, THERMODYNAMICS AND KINETICS OF METALLIC NANOALLOYS

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The technological application of nanoalloys (NAs), agglomerates of two or more transition metals with a diameter of less than few tens of nanometers, is constantly growing in various fields ranging from catalysis to magnetic storage and biomedical uses. For those applications, the design the NA with the targeting property is highly desirable. Due to their peculiar surface and bulk geometries, which strongly influence the electronic structure, and to the richness of structures and mixing patterns nanoalloys exhibit, numerical simulation tools can give insights on which should be considered the 'best structural motif'. Moreover, since the synthesis- structure-performance relationships have not been elucidated yet, atomistic modelling can help in driven experiments. In this talk, we will show how the molecular dynamics tool, both at classical and *ab-initio* level of theory, can be used in order to characterize the energetic and thermal stability of metallic nanoalloys. Finally, the modelling of the growth of nanoalloys is discussed from an atomistic point of view, where atom-by-atom growth molecular dynamics simulations have been used to identify different formation patterns, ranging from core/shell to Janus motifs.

O1

A FIRST PRINCIPLES STUDY OF POINT DEFECTS AND SITE OCCUPANCY IN $D8_m$-Nb_5Si_3, $D8_l$-Nb_5Si_3, $D8_m$- Mo_5Si_3

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Keywords: First-principles; Defect enthalpies of formation; Site preference; Nb_5Si_3; Mo_5Si_3

First principles calculations of point-defect enthalpies of formation were performed in the $D8_m$-Si_3Nb_5, $D8_l$-Si_3Nb_5, and $D8_m$-Si_3Mo_5 compounds [1]. Four sublattices are introduced to account for the $D8_m$ as well as for the $D8_1$ structure. To determine the defect formation energies, the ab-initio calculations were performed on a 1x1x2 supercell of 64 sites in the case of the $D8_m$ structure and on a 1x1x1 supercell of 32 atoms in the case of the $D8_l$ structure.

Based on a statistical-thermodynamic model which is an extension to four sublattices of the model proposed by Hagen and Finnis [2], the defect concentrations were calculated as function of temperature and deviation from stoichiometry in each compound. These calculations have allowed to show that the off-stoichiometry of the $D8_m$-Nb_5Si_3 and $D8_m$-Mo_5Si_3 compounds in the Si-rich side is due to the presence of Si antisites on the Nb or Mo 4b sites of the $D8_m$ structure.

The site preference of B and Mo in $D8_m$-Si_3Nb_5, $D8_l$-Si_3Nb_5, and B and Nb in $D8_m$-Si_3Mo_5 has also been studied. The site preference of Mo in $D8_m$-Si_3Nb_5 and $D8_l$-Si_3Nb_5 is the Nb sites. The site preference of B in $D8_m$-Si_3Nb_5 and $D8_m$-Si_3Mo_5 is the Si sites. The site preference of B in $D8_l$-Si_3Nb_5 is the 8h Wyckoff positions occupied by Si atoms of the $D8_l$ structure.

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O2

PHASE EQUILIBRIA AND PHASE TRANSFORMATIONS IN Fe-Mn BASED ALLOYS

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Phase equilibria between α (ferrite) and γ (austenite) in the Fe-Mn based alloys are briefly reviewed [1,2], focusing on the temperature dependence of the partial molar free energy change of Mn between α and γ phases [3], the peculiar shape of the γ-loop formed in the Fe-Mn-X (X: ferrite stabilizing element) and the Ni-equivalent of Mn in the Schaeffler diagram. The characteristic features of α/γ equilibria of Fe-Mn based alloys result in martensitic transformation from the ferrite to the austenite phase observed in the Fe-Mn-Al system [4]. The origin of this unique transformation and the superelastic properties accompanied by martensitic transformation in the Fe-Mn-Al-Ni alloy [5] are also shown.

Finally, the thermodynamic database of the Fe-Mn based alloys, including the elements of C, Al, Si and Cr developed by CALPHAD approach is shown. The design of high-strength, low-density alloys using this database is presented [6].

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O3

PHASE RELATIONS AND MELTING BEHAVIOR IN CLATHRATE SYSTEMS $BA_8\{CU,AG,AU\}_X\{SI,GE\}_{46-X}$

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Keywords: Clathrate type-I; Crystal structure; Phase equilibria; Liquidus projection

Formation and homogeneity range of the ternary clathrates of type-I, $Ba_8\{Cu,Ag,Au\}_x\{Si,Ge\}_{46-x}$ (space group Pm-3n) at 800°C and phase relations concerning this region have been investigated. For all the ternary systems, Ba-Cu-Ge, Ba-Cu-Si, Ba-Ag-Ge, Ba-Ag-Si, Ba-Au-Ge and Ba-Au-Si, partial isothermal sections have been derived at 800°C for the region of 0 to 33 at% Ba. For characterization of the clathrates and other ternary compounds existing at 800°C, X-ray powder diffraction (XRD), electron probe microanalysis (EPMA) and X-ray single crystal diffraction were used.

For the Ba-Ag-Ge system, also the liquidus and solidus projection has been constructed up to 33.3 at.% Ba, using EPMA, XRD and differential thermal analysis (DSC/DTA). Eight different primary crystallization regions were found: (Ge), $Ba_8Ag_xGe_{46-x-y}\square_y$ (κ_I) ($\square$ is a vacancy), $Ba_6Ag_xGe_{25-x}$ (κ_{IX}), $BaGe_2$, $Ba(Ag_{1-x}Ge_x)_2$ (τ_1), $BaAg_{2-x}Ge_{2+x}$ (τ_2) $BaAg_5$ and (Ag). The ternary invariant reactions have been determined for the region investigated and are the basis for a Schulz-Scheil diagram.

O4

APPLICATIONS OF CDCVM TO THE STUDY OF ALLOY PHASE EQUILIBRIA

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Phase Cluster Variation Method (CVM) has been recognized as one of the most reliable statistical mechanics methods to the study of alloy phase eqilibria. However, one serious drawbacks of the CVM stems from the fact that the local atomic distortion is by no means introduced in the free energy formula. Hence, the resulting free energy minimum does not guarantee that the system is in a fully equilibrium state. This is particularly so for a disordered phase in which atomic species with different sizes have more chances to encounter. In order to circumvent such inconveniences, Continuous Displacement Cluster Variation Method (CDCVM) has been developed. For the CDCVM, a certain number of additional points to which an atom can be displaced are introduced around each Bravais lattice point, and these points are termed quasi-lattice point. And atoms displaced to different quasi lattice points are regarded as different atomic species locating at a Bravais lattice point. This way, the local lattice distortion is mapped onto the phase equilibria of a multi-component alloys system. By employing CDCVM, we calculated phase diagram, atomic distribution around a Bravais lattice point, diffuse intensity spectrum due to the local distortion etc. We also extended the CDCVM to the study of displacive phase transformation.

O5

ENTHALPIES OF FORMATION AND SPECIFIC HEAT OF SELECTED HEUSLER ALLOYS Ni_2XY (X = Zr, Hf, V, Nb, Ta, Mn; Y = Al, In, Si, Sn)

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Keywords: Enthalpy of formation; Specific heat; Heusler Alloys; Calorimetry; Ni_2XY

The enthalpies of formation and specific heat of selected ternary Heusler alloy compositions Ni_2XY (X=Zr, Hf, V, Nb, Ta, Mn; Y=Al, In, Si, Sn) were measured by high temperature reaction calorimetry and drop calorimetry. The lattice parameters of the compounds with $L2_1$ structure were determined and impurity phases were analyzed using optical microscopy and energy dispersive spectroscopy. The x-ray diffraction patterns were simulated using CrystalMaker and CrystalDiffract in order to confirm the phases present and estimate the phase fractions. The compounds $AlNbNi_2$, $AlNi_2Ta$, $AlNi_2V$, $AlNi_2Zr$, $GeMnNi_2$, $HfInNi_2$, $InMnNi_2$, $MnNi_2Si$, $MnNi_2Sn$ were determined to exist in the $L2_1$ structure. The enthalpies of formation for these compounds were determined to be -38.9±1.5, -38.7±1, -39.7±0.5, -50.2±2.5, -21.0±1.9, -34.7±2.8, -21.6±2.8, -29.3±2.5, -19.1±4 kJ per mole atoms, respectively.

O6

EXPERIMENTAL INVESTIGATION OF PHASE EQUILIBRIA AT LOW TEMPERATURES (< 600°C) IN THE Fe-Ni BINARY SYSTEM

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In the Fe-Ni system, interesting phase equilibria at low temperatures below 600°C have been proposed by experimental studies and predicted by thermodynamic calculations. For instance, the existence of the Nishizawa horn along the Curie temperature of the fcc γ (Fe, Ni) solution phase and that of the ordered γ''FeNi ($L1_0$) phase were suggested by experimental investigation on meteorites [1] and predicted by the CALPHAD [2] and *ab-initio* [3] calculations. Furthermore, it was reported that the solubility of Ni in the α Fe shows “retrograde solubility”, *i.e.*, the Ni solubility increases with decreasing temperature below A_3 point of pure Fe and starts decreasing again below 500°C until the invariant reaction, γ (Fe, Ni) => α Fe + γ' Ni_3Fe ($L1_2$). The solubility of Ni in the α Fe at low temperatures below 500°C was determined by Goldstein *et al.* [4], Romig *et al.* [5] and Zhang *et al.* [6], in which small particles of γ (Fe, Ni) precipitated in α' Fe martensite matrix were examined by XRD, EPMA, TEM, *etc.* However, it seems that extra energies due to the martensite structure might cause the deviation of the solubility limit from the true equilibrium composition, especially at low temperatures. In this study, extremely deformed particles of the Fe-Ni alloys were equilibrated at low temperatures below 600°C and phase equilibria were determined by a FE-EPMA (JEOL:JXA-8500F) with high special resolution (< 1 μm).

Gas-atomized powders of Fe-Ni alloys were prepared and deformed extremely by converge milling method. Each powder sample was encapsulated in an evacuated quarts capsule and equilibrated at temperatures between 400 and 700°C for various durations up to 3 months. After that, each sample was molded in a conductive resin, mechanically polished, and finished by a vibratory polisher with 0.1 μm diamond suspension. Microstructures of the powder samples were examined and equilibrium compositions were determined by the FE-EPMA with low accelerating voltage of 6 kV.

Dual-phase structures consisting of strain-free particles of the α Fe and γ (Fe, Ni) phases, whose grain size reached up to 1 μm, were obtained after heat-treatment above 400°C for 3 months. Results of experiments suggest that the equilibrium compositions of the γ (Fe, Ni) are in consistent with the previous data in the literature. However, it was confirmed that the Ni solubility in the α Fe increases monotonously with decreasing temperature, which suggests that the “retrograde solubility” seems to be incorrect in the Fe-Ni system.

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O7

PHASE EQUILIBRIA OF THE PARTIAL SYSTEM CoSiTi – Ti_5Si_3 – TiSi – $Co_4Si_7Ti_4$

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The subsystem CoSiTi – Ti_5Si_3 – TiSi – $Co_4Si_7Ti_4$ is the high melting region in the Co-Si-Ti ternary system. This causes substantial difficulties to obtain equilibrated alloys by annealing at temperatures as low as 1000°C as well as to determine the melting temperatures, which are at 1490°C and higher. Despite the ternary boundary phases CoSiTi and $Co_4Si_7Ti_4$ two ternary phases are observed in the composition region of the current interest: The previously reported phase „$CoSi_4Ti_4$“ [1] at compositions 12-13 at% Co, 43-44 at% Si and 43-44 at% Ti and a newly discovered phase $Co_{17}Si_{40}Ti_{43}$, which is isostructural to the phase τ_8 of the system Fe-Si-Ti [2]. A partial isothermal section, a projection of the corresponding segment of the liquidus surface, as well as a reaction scheme linking these two will be proposed.

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LIQUID PHASE SEPARATION, SOLIDIFICATION AND PHASE TRANSFORMATIONS OF Gd-Ti AND Gd-Ti-Al-Cu ALLOYS

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Phase separated metallic glasses can be produced from complex alloys involving binary terminal systems with both negative and positive heats of mixing. Here we consider Gd-Ti based systems with a positive heat of mixing $\Delta H_{m,Gd-Ti}$= + 15 kJ/mol. Droplets of the reactive melts were investigated by the electromagnetic levitation technique. The effect of melt undercooling prior solidification was revealed from microstructure analysis of quenched samples. Phase transformations were studied by differential scanning calorimetry (DSC).

For binary Gd-Ti alloys a liquid miscibility gap, ranging from 10 to 80 at.% Gd was identified from the coarse phase separated microstructures [1]. The critical temperature $T_c \approx$1580°C of the binodal curve is near the composition $Gd_{20}Ti_{80}$. According to Chang et al.[2] metallic glasses of quaternary Gd-Ti-Al-Co/Cu alloys with unique spinodally decomposed microstructures can be produced by melt spinning.

Using the CALPHAD method a miscibility gap and a spinodal curve in the quaternary systems have been predicted. Because the thermodynamic data is rather scarce experimental investigations for various alloys on the section $Gd_{55-x}Ti_xAl_{25}Cu_{20}$ (x = 0 to 55) have been accomplished.

The DSC data at a heating rate of 20 K/min exhibit various phase transformations of the rather complex alloys. There is an obvious drop of liquidus temperatures from $T_{liq} \approx$1120 to 1150°C for Ti-rich (x >10) alloys to $T_{liq} \approx$ 950°C for Gd-rich ($x \leq$ 10) compositions, respectively [3]. This is connected with a change of the primary solidification from α-Ti toward a Gd_2AlCu-type phase (50.8Gd-28.5Al-20.7Cu; at.%). The microstructure of quenched droplets for melt undercoolings up to $\Delta T = T_{liq} - T \approx$200 K was investigated. However, no indication of liquid phase separation was detected even for a $Gd_{25}Ti_{30}Al_{25}Cu_{20}$ sample quenched from 920°C, at the experimentally accessible temperature limit, which is well below the spinodal line calculated by the CALPHAD method. Instead a dramatic coarsening of the α-Ti dendrites with increasing ΔT was observed. Therefore, we suspect that the fine-scaled microstructures observed in rapidly quenched ribbons[2] may be due to spinodal composition in the glassy state.

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O9

EXPERIMENTAL STUDY AND THERMODYNAMIC REMODELLING OF THE TERNARY Ti–Al–C SYSTEM

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Gradually increasing interest to the Ti-Al-C system is related with development of materials based on γ-phase (TiAl) as well as on the Ti_2AlC and Ti_3AlC_2 ternary compounds or so-called MAX-phases. The MAX-phases possess unique properties combining merits of both, metals and ceramics. It is also well known that additions of titanium carbide (TiC_{1-X}) particles refine grains of Al alloys enhancing their properties. The TiC_{1-X} has prospects to be applied as a reinforcing phase in Ti-, Al-based and γ-TiAl alloys, as well as a hard constituent of Ti- an Al-matrix composites.

Many works were dedicated to the investigation of the Ti-Al-C system and their data were recently assessed in [1]. However, data on phase equilibria in the range of melting/solidification of alloys are scarce and those reported in the literature phase transformation temperatures are contradictory.

In the present work a thermodynamic CALPHAD-type description of the ternary Ti–Al–C system[2] was remodelled based on novel experimental information from literature and own experimental results. Dedicated experiments were performed in order to complement literature data on phase equilibria, especially in the range of melting/solidification. To this end twelve key samples containing up to 25 at.% C were prepared by arc melting with non-consumable tungsten electrode, annealed at sub-solidus temperatures (by 30-60 K lower than the temperature of incipient melting) and analyzed by means of XRD, DTA and SEM/EDS/EBSD techniques in as-cast and annealed states.

The elaborated thermodynamic description was applied to calculate selected phase equilibria as to provide a comparison between calculated and experimental results. The calculations are shown to reproduce reasonably the experimental data.

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O10

INTERACTION OF RARE EARTH ELEMENTS WITH Cd: THERMOCHEMISTRY AND PHASE EQUILIBRIA IN THE SYSTEMS Cd-Nd AND Cd-Ce

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Many countries in the world have strong and effective nuclear programs to become independent of foreign energy sources, producing an ever increasing amount of nuclear waste. Suitable recycling and safe disposal of this waste is therefore a key issue to allow for a continuous use of nuclear energy. A number of different techniques are currently under development for the recycling of spent fuel rods, and one of them is a pyrochemical separation technique[1]. A central process in it is the electro-refining step where, in particular, rare earth (RE) metals are extracted from spent fuel rods with Cd in an electrochemical cell. The RE metals form intermetallic compounds with Cd and accumulate at the bottom of the cell. The extraction behavior is primarily affected by the stability of these compounds, and thus a thorough knowledge of existence and stability of intermetallic compounds in the various binary systems Cd-RE is highly important.

Literature information on the phase diagrams of the two systems Cd-Nd and Cd-Ce is very limited[2], and not much is known about the thermodynamic properties of the two alloy systems. Therefore, it is the aim of the present study to clarify phase equilibria in the Cd-Nd and Cd-Ce system (and to confirm available literature information) by means of powder X-ray diffraction (XRD), differential thermal analysis (DTA) and electron probe microanalysis (EPMA). Additionally, an isopiestic vapor pressure method is applied to determine partial thermodynamic properties of Cd. These experiments are supported by measurements of the electromotive force (emf) using a molten salt electrolyte, from which also partial thermodynamic properties can be derived allowing a valuable cross-check of experimental results.

All experimental results together with the available literature information will be used as input in a CALPHAD-type optimization of the two systems.

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O11

FIRST PRINCIPLES MODELING OF FORMATION AND STABILITY OF FCC-NdO_X AT Nd/Nd-Fe-B INTERFACE

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The development of advanced Nd-Fe-B permanent magnet materials with high coercivity draws the high attention of researchers on the relation between coercivity and structure at the grain boundaries. A disordered fcc-NdO_x phase formed at the interface of Nd/Nd-Fe-B is observed and it is believed to take an important role in coercivity generation [1,2]. To have a thorough understanding on the formation mechanism of this particular oxide phase, ground state analysis for a whole oxygen concentration in Nd-O has been performed. Based on LSDA+U calculations for selected ordered phases at various oxygen concentrations, properties of the disorder NdO_x phase can be further evaluated combing with the Cluster Expansion Method (CEM) [3]. It is shown that at low oxygen concentration, the system tends to separate into dhcp-Nd and NaCl -NdO or ZnS -NdO, whereas at oxygen concentration over 50%, the Nd_2O_3 becomes most stable. Based on the stability analysis, a formation model on fcc-NdO_x is proposed along a sequent structures from Fluorite-NdO_2, C-type(cI80)-Nd_2O_3 to ZnS-NdO which have same fcc-frame of cations and vary in configurations of oxygen anions due to introducing oxygen vacancies. Formation energies, electronic structures are calculated for various oxygen vacancies configurations, which revealed the formation mechanism of this fcc-base phase developed at the interface between $Nd_2Fe_{14}B$ and hcp-based Nd-rich matrix. The interface calculation of NdO_x/Nd clarified the origin of the stability of this fcc-based oxide phase on Nd metal.

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O12

EXPERIMENTAL AND THERMODYNAMIC ASSESSMENT OF THE Gd-Zr AND Gd-Ti PHASE DIAGRAMS

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The phase equilibria of the binary Gd-Zr and Gd-Ti system have been investigated by means of in situ synchrotron high energy X-ray diffraction at elevated temperatures up to 1900 K. An electrostatic levitator has been used specially designed for scattering experiments of metallic liquids. The container-less method ensured the avoidance of any reactions between the melt and crucible materials. The in situ X-ray diffraction enabled a direct measurement of the coexistence ranges and the occurrence of phase transformations as a function of temperature. The temperature dependence of diffraction patterns of the liquid phase was analysed in detail. From the data the liquidus line of the Gd-Zr and Gd-Ti phase diagrams could be assessed. Based on the experimental data improved Gd-Zr and Gd-Ti phase diagrams were derived and a thermodynamic description of the binary systems was developed. The importance of the knowledge of the phase diagrams for the understanding of the structure formation of Gd-Zr and Gd-Ti based phase separated metallic glasses is pointed out.

O13

THERMODYNAMIC CHARACTERIZATION OF ALUMINIUM CORNER OF Al-Cu-Nd

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Keywords: $AlCu_5Nd$ alloy; Thermodynamics; Solidification; Thermal analyses

The aluminum corner of ternary system Al-Cu-Nd was investigated using simple thermal analysis, calculations of thermodynamic equilibrium, differential scanning calorimetry (DSC) and optical and scanning electron microscopy (SEM). The phase Al_2Cu became rich on the neodymium and formed a new eutectic (α_{Al} + $Al_2Cu(Nd)$). By increasing the content of Nd, the amount of eutectic phase Al_2Cu and consequently eutectic itself in the microstructure is increased.The temperature of eutectic solidification (α_{Al} + Al_2Cu) also moves to higher temperature whereas the recalescence disappears even at a small amount of Nd. The solidification time interval is widened when 0.1−1 wt. % Nd is added and narrowed when 5 wt. % of Nd is added. The solidification of specimen with highest Nd content ends at higher temperature as the solidification of specimens with lower Nd content.

O14

WETTABILITY AND INTERFACIAL REACTIONS IN THE (Ni,B)/ZrB_2 SYSTEM

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Keywords: Wetting; borides; Nickel alloys; CALPHAD; Interfaces

Ti, Zr and Hf diborides are ideal materials for advanced high temperature applications because of their high melting point, chemical inertness, thermal and electrical conductivity, hardness and thermal shock resistance. In order to obtain tough and reliable ceramic/ceramic joints, wettability studies of diborides by brazing alloys are mandatory. This group has already undertaken a systematic study of wettability, reactivity and interfacial properties of several alloy / diborides systems: (Cu, Ag, Au) / ZrB_2 [1], (Cu, Ag, Zr) / ZrB_2 [2], Ni-B / ZrB_2 [3] and Ni-B / HfB_2 [4].

In this work sessile drop experiments performed in the Ni-B/ZrB_2 system are presented; they show that in the range 1110° ≤ T ≤ 1150° C a peculiar and to our knowledge not yet reported phenomenon takes place, namely isothermal solid-liquid transitions occur reversibly at the alloy/ceramic interface. This complex behaviour has been studied and interpreted on the basis of the B-Ni-Zr phase diagram computed by CALPHAD [5], setting a link between wetting and joining experiments and phase diagrams assessment.

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O15

GRAIN BOUNDARIES ON THE SURFACE OF MgO AS A PRECURSOR FOR IMPROVED CATALYTIC ACTIVITY: DFT STUDY

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Keywords: Grain boundaries; Density Functional theory; Catalyses

Polycrystalline metal-oxide materials find numerous technological applications where grain boundaries (GB) are known or suspected to influence functionality. A large number of experiments demonstrate clear evidence that GB in MgO act as sinks for defects, impurities and also can provide shortcut paths for their diffusion. Low-coordinated ions in GB areas of MgO nanocrystals were recently considered as acid-base sites for catalyses. To get knowledge about the fine structure of GB and to put light on the changes in bonding in the vicinity of disordered regions near GB the *ab initio* calculations may be useful.

Density Functional theory (DFT) is applied to study the atomic structure of high angle GB in the nanocrystaline MgO. Relaxation of the atomic layers in the vicinity of the interface between nanocrystals was calculated by minimizing the forces applied to the ions in the supercell consisted of regular crystal cells and GB. The performed investigation shows that the relaxation in the vicinity of GB penetrates inside the grain to the distance that does not exceed 3-4 atomic layers from GB: the change in the relaxation energy fades and the average atomic displacements decrease in such a way that at the third atomic layer the relaxed and non-relaxed atomic positions differ not higher than 3% of the lattice parameter. Analysis of the Density of States for electrons shows the existence of additional states in the band gap close to the bottom of the conduction band. This may serve as a precursor for increasing the adsorption properties.

O16

PHASE-FIELD SIMULATIONS OF THE SOLIDIFICATION OF HYPOEUTECTIC Al-Si CAST ALLOY BASED ON THERMODYNAMIC AND CHEMICAL MOBILITY DATABASES

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Hypoeutectic Al-Si alloyed by Mg and Fe is widely used as cast alloy. Minor addition of Sr is known to essentially change the eutectic morphology. In the 'unmodified' state without Sr, Al-Si alloys exhibits an irregular eutectic structure with interconnected flake-shaped silicon. Addition of Sr results in a 'modified' eutectic morphology characterized by fine fibrous silicon, more favorable for mechanical properties. However, it is frequently observed that modified and unmodified regions coexist in the microstructure of the same casting, a usually undesired phenomenon known as 'heterogeneous modification'. A possible explanation is that the formation of Sr containing precipitates, in particular Al_2Si_2Sr, leads to local depletion of Sr in the melt at the onset or during the eutectic transformation. Phase-field simulations are performed to provide a basis for quantitative discussion of this hypothesis.

Microstructure simulations are performed for the alloy Al-7%Si-0.3%Mg-0.1%Fe-0.025%Sr using the phase-field software Micress®. The thermodynamic data for the multiple phase interactions are calculated from a Calphad database by online-coupling to the TQ interface of the ThermoCalc® software. Additionally, a chemical mobility database is coupled to evaluate the diffusion coefficients of the multiple solutes in the various phases. Simulations are run under variation of process parameters and nucleation conditions to study the effect of Al_2Si_2Sr precipitation on the Sr distribution. A first series of simulations are run until the onset of the eutectic transformation in order to evaluate Sr distribution maps at the stage of primary silicon precipitation. Further simulations follow the eutectic transformation until the end of solidification. The effect of Sr on the morphology of eutectic silicon is modeled by an effective anisotropy formulation. This formulation bridges the scale from the internally twinned structure of silicon, too fine to be resolved in practical computations, to its outer lamellar appearance, which thus evolves in the phase-field simulation as either flake-shaped or fibrous.

O17

CRITICAL THERMODYNAMIC EVALUATION OF THE Pb-Sb SYSTEM INCLUDING EQUILIBRATION TESTS TO DETERMINE SOLID SOLUBILITIES OF LEAD IN ANTIMONY AND VICE VERSA

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The Antimony-Lead phase diagram comprises of a simple Eutectic system, of which especially the properties of the liquid phase and the compositions of the liquidus lines on both sides have been extensively studied. The liquid phase is characterised by almost Raoultian behaviour.

Whilst the face centred cubic Lead rich phase has been relatively well defined by measurements in both solidus and solvus, the rhombohedral Antimony rich phase is not very well established (because the measured data is widely scattered). The solvus does not appear to be measured at all and the phase diagram at this particular spot is thus just extrapolated by continuation of solidus measurement data, which is a very crude estimation.

Most of the data present for both solidus and solvus in literature was measured by dynamic methods, such as differential thermal analysis (DTA) and differential scanning calorimetry (DSC). With those a true equilibrium cannot always be reached, because a reasonable measurement resolution for those methods requires a certain minimum temperature scan rate.

Especially for solids the mobility of atoms is quite limited and a true equilibirum thus not easily realised. To prevent non equilibrium results, equilibration tests can be conducted, where after the sample is quenched and the solubility is measured by determining both compositions in a 2 phase mixture using electron microprobe analysis (EPMA).

This work seeks to improve the quality of the data available for solidus and solvus lines in the Lead-Antimony system and generate an improved phase diagram evaluating the measured results and the thermodynamic data already available in literature.

O18

ELECTRICAL CONDUCTIVITY AND ENTHALPY OF MIXING OF Co-Sn LIQUID ALLOYS

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Keywords: Co-Sn; Enthalpy of mixing; Electrical conductivity; Thermo-e.m.f. ; High temperature

The Co-Sn system is of considerable technological importance. The phase relations and thermodynamic properties have been repeatedly investigated by several authors. However, a large discrepancy between different experimental data of enthalpy of mixing exists, e.g. the $\Delta_{mix}H$ versus x_{Co} curve generally shows endothermic or exothermic mixing behavior or both effects dependent on concentration. Literature data have been measured at different temperature but no systematic and reasonable change with temperature can be observed. At the same time, no electrophysical data of the Co-Sn alloys in the liquid state were reported. The knowledge of the electrical conductivity and the thermo-e.m.f. behaviour and their influence on the interactions between structural units is important to understand the mechanism of a charge transport.

The aim of this work was first to determine the enthalpy of mixing of liquid Co-Sn alloys at temperatures from 400 – 1300 °C in steps of 100 K using the drop calorimetric method. Furthermore, thermoelectric properties of liquid Co-Sn alloys have been determined and compared to the enthalpy of mixing. The electrical conductivity and thermo-e.m.f. were measured in the concentration range between 0-60 at.% Co. The enthalpies data, obtained at a constant temperature of 973 K, are compared with literature data. Based on the obtained results an interaction between unlike atoms with possibility of the associate formation has been suggested.

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O19

PHASE DIAGRAM OF THE Al-Ge-Ti SYSTEM

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The phase diagram Al-Ge-Ti is of potential interest for joining applications for titanium-aluminides which are important alloys for high temperature components. Aluminum and Germanium form a deep eutectic (420°C) which could be used for soldering of titanium-aluminides in the transient liquid bonding process. A thorough knowledge of ternary phase equilibria is required for the realization of interface reactions during bonding and the search for possible ternary Al-Ge-Ti alloys that could be employed as solders. However, up to now the Al-Ge-Ti phase diagram was not studied.

In this work the phase equilibria of Al-Ge-Ti have been investigated using scanning electron microscopy (SEM), powder x-ray diffractometry (XRD) and differential thermal analysis (DTA) measurements in order to obtain partial isothermal sections at 400°C, 520°C and 1000°C. Different annealing temperatures in different parts of the system were necessary because of the strongly varying melting points (between 420°C and 1980°C). Two ternary and one new binary compounds were found to exist, two of which could be structurally characterized ($Al_{0.10-0.24}Ge_{0.42-0.56}Ti_{0.33}$, $Al_4Si_5Zr_3$-typ, $I4_1/amd$, $tI24$) ($Ge_{44}Ti_{56}$, Ge_4Sm_5-typ, *Pnma*, $oP36$). DTA data were used to construct a ternary reaction scheme (Scheil). Also, preliminary brazing experiments were performed in order to test the wetting behaviour and interface reactions.

O20

ORDERING PHASE RELATIONS IN TERNARY IRON ALUMINIDES

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Keywords: Cluster Variation Method; Iron aluminides; *Ab-initio* calculations

One of the key issues in the development of iron aluminides is the thermodynamic modelling of alloying effects on the long-range and short-range order states of the underlying BCC phase, needed for the proper description of their effects upon phase equilibria in the multicomponent alloys. The present work describes results obtained by the present research group in the development of a thermodynamic database using the cluster variation method (CVM) in the irregular tetrahedron approximation, combined with ab-initio results obtained from FP-LAPW electronic structure calculation in the GGA approximation, as embodied in the Wien2k package. The ordering phase equilibria in isothermal sections of systems Fe-Al-Mo, Fe-Al-Nb and Fe-Al-Ti are compared. These equilibria, particularly in the technologically important iron-rich corner, are characterized by radically different behaviours, ranging from unlimited solubility of Ti in the $D0_3$ and B2 phases, to a very small solubility of Mo in these two phases. The behaviour of Nb is somewhat intermediate between these two extremes, and show a limited solubility in the B2 phase, which is, however, found in equilibrium with a stable $D0_3$ phase. It can be shown that these different behaviours can be understood as a consequence of the different metastable equilibria in the binary Fe-Mo, Fe-Nb and Fe-Ti systems. The results, particularly in the case of Fe-Al-Nb, are discussed in reference with experimental data on the stable and metstable ordering equilibria in these systems.

O21

THE EXPERIMENTAL AND THEORETICAL STUDY OF THE In-Ni-Sn SYSTEM

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The phase diagram of the In-Ni-Sn system was studied experimentally and modeled theoretically in this study. Isothermal sections of the phase diagram were determined experimentally at 400 and 700 °C using long-term annealing SEM-EDX, and DSC/DTA measurements in order to determine phase transition temperatures. The coexisting phases were further defined using X-ray diffraction methods. At least two new ternary compounds existing at 400 °C and one ternary phase at 700 °C were found and their crystal structures were determined. All compounds exhibit already known crystal structure types.

All experimental data were used together with other experimental data from literature for the complete assessment of the In-Ni-Sn system. Very good agreement was reached between the experiment and theoretical calculations.

The theoretical assessment is very useful for the development of materials suitable for lead-free soldering, as it allows modeling of the processes at low temperatures, important for practical applications.

O22

THERMODYNAMIC PROPERTIES OF THE TERNARY LIQUID Ag-Cu-Ga SYSTEM

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Keywords: Thermodynamics; Trnary system; Gallium alloys; E.M.F. ; Calorimetry

Using calorimetric and E.M.F. methods, thermodynamic properties of the liquid Ag-Cu-Ga system were investigated. Consequently, drop calorimetric measurements were carried out along the following cross-sections:

-X(Ag)/X(Ga) = 1:1 at two temperatures 1123 and 1273 K

- X(Cu)/X(Ga) = 1:1 at two temperatures 1123 and 1273 K

and integral enthalpies of mixing of liquid ternary alloys were determined at those temperatures.

Next, E.M.F. measurements were done using solid oxide galvanic cells with zirconia electrolyte. The E.M.F.'s of the cells

$Ag_xCu_yGa_{1-x-y}$, Ga2O3 //$ZrO_2 + Y_2O_3$// Fe, FeO (I)

were measured in the temperature range from 1023 to 1273 K for three cross-sections X(Cu)/X(Ag) = 3:1, 1:1 and 1:3.

All the data taken together with the information about binary systems were used to describe thermodynamic properties of liquid alloys.

O23

THE STANDARD ENTHALPIES OF FORMATION OF SOME BINARY INTERMETALLIC COMPOUNDS OF LANTHANIDE – IRON SYSTEMS BY HIGH TEMPERATURE DIRECT SYNTHESIS CALORIMETRY

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The standard enthalpies of formation of intermetallic compounds of some Lanthanide-iron systems have been measured by high temperature direct synthesis calorimetry at 1373 ± 2K. The following results in kJ/mole of atoms are reported: Ce_2Fe_{17}(-1.6 ± 2.8); Pr_2Fe_{17}(-0.2 ± 3.0); Nd_2Fe_{17}(-3.0 ± 2.7); Sm_2Fe_{17}(-3.1 ± 3.2); $GdFe_2$(-2.4 ± 3.0); $HoFe_2$(-2.6 ± 3.3); $ErFe_2$(-1.9 ± 3.0); $TmFe_2$(-2.2 ± 2.8); $LuFe_2$(-3.6 ± 3.1).

The standard enthalpies of formation of some binary and ternary shape memory alloys have also been measured. These are: Terfenol-D(-1.5 ± 3.1), Samfenol(-13.6 ± 3.1), Galfenol(-10.4 ± 2.8).The values are compared with predicted values of the semi empirical model of Miedema and Coworkers and with predictions by *ab initio* calculations. We will present a systematic picture of how the enthalpies of formation may be related to the atomic number of the Lanthanide element. We will also compare the thermochemical behavior of LA-Ni and the LA-Fe alloys.

O24

PHASE TRANSFORMATIONS AND THERMODYNAMIC DESCRIPTION OF Al-Sb-Zn ALLOYS

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Keywords: Al-Sb-Zn; DTA, Phase Transformations; Enthalpy of Mixing

DTA heating curves were calculated and compared to the experimentally recorded ones for the purpose of the phase transformation study of Al-Sb-Zn ternary alloys. The calculations were done on the basis of the Boettinger and Kattner model [1]. The thermodynamic parameters were taken from SSOL4 database. On the basis of the description of the thermodynamic properties of the binaries [2, 3, 4], the isopleths and isotherms were calculated and compared with the existed one [5, 6]. Liquid alloys were studied through the predicted thermodynamic properties and the measured enthalpy of mixing at 1080 K.

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O25

THE THERMODINAMICS AND SURFACE PROPERTIES OF LIQUID Si-Ge ALLOYS

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Thermophysical properties of liquid state of semiconductors (Si, Ge) are interesting form both technological and scientific prospectives. From the technological point of view, knowledge of the thermophysical properties is necessary for growing better single crystal. On the other hand, from the scientific prospective, knowledge of the temperature dependence of these properties will provide information on metallic-to-semiconductor transition associated with the structural change in the liquid and its correlation with the above mentioned properties.

However, despite of the importance of these properties, the characterization of the thermophysical properties of such metallic systems is hampered by the experimental difficulties due to the high melting temperatures of Si-rich alloys, and the high reactivity of these metals with ceramic materials. In this work, we aim at presenting the experimental data obtained for the surface tension of the three Si-Ge liquid alloys compared with thermodynamic models. Instead of the traditional techniques, as sessile drop or large drop, we employed the quasi-containerless technique of the pendant drop in order to reduce the contact between the ceramic material of the container and the liquid metal.

The surface tension measurements have been performed on the three alloys with the following compositions: Si-25Ge, Si-50Ge, Si-75Ge (in at.%) and on the pure components. For each sample, the surface tension has been measured as a function of temperature in a wide range above the corresponding liquidus temperature.

The observed behaviour, with respect to both, temperature and concentration, has been compared with thermodynamic model calculations using the regular solution approximation (REG) and the ideal solution model.

O26

DENSITY AND VISCOSITY OF LIQUID Al-Cu-Si ALLOYS

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Keywords: Al-Cu-Si liquid alloys; Density, Electromagnetic levitation; Thermophysical properties; Viscosity

The Al-Cu-Si alloy system is the basis for many commercially used lightweight alloys, in particular, in the automotive or aerospace applications. Nevertheless, surprisingly few data exist regarding the thermophysical properties of the liquid phase. Here, we report on density and viscosity measurements; properties which are fundamental for both technical applications and a general characterization of a system.

Densities have been measured using the non-contact technique of electromagnetic levitation. A CCD camera records a series of side view shadow images. The volume, from which the density was derived, was calculated afterwards from an average of the profile lines. It was found that the density was a linear function of temperature for all investigated compositions. In order to describe the concentration dependency, only a negligibly small excess volume ^{E}V could to be taken into account for the ternary Al-Cu-Si alloys even though the binary margin phases Al-Cu and Cu-Si require $^{E}V<0$.

Viscosities of Al-Cu were obtained in oscillating cup viscometry. This method employs a crucible containing the liquid sample suspended by a torsion wire. The crucible performs angular oscillations which are damped by the inner friction of the liquid. Viscosities are calculated from the time period and the decay of the amplitude by solving the Roscoe equation. The temperature dependence can be described by an Arrhenius law, taking into account activation energies for the viscous flow. Depending on concentration, both viscosity and activation energy show an extremum corresponding to the existence of intermetallic phases. The results are compared to model calculations.

O27

NOVEL GROWING INTERMEDIATE PHASES IN Ni/Al DIFFUSION-REACTION COUPLES

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Keywords: Kinetics; Intermetallics; Al-Ni; TLPB; Microhardness

The Ni-Al system has been intensively studied since several years because its intermediate phases (IP) presented interesting properties from basic and technological point of view [1]. There is a wide range of industrial applications for these IPs, from corrosion withstanding coatings to turbine blades. The formation of Al-Ni IPs is analyzed in the multilayer system obtained by means of Transient Liquid Phase Bonding (TLPB) process [2]. Therefore this work presents the kinetic and physicochemical characterization of the growing IPs layers of the Ni/Al couples between 720 to 1170ºC, in particular the Ni-rich side.

The results showed the presence of 5 IPs layers instead of the 4 predicted by the equilibrium phase diagram [3]: C1: Al_3Ni, C2: Al_3Ni_2, C3: AlNi-rich, C4: AlNi-poor and C5: $AlNi_3$. In accordance with the findings of others authors [4-6], this additional layer C4 may correspond to Al_4Ni_3. Interdiffusion coefficients for the growth of this layers and microhardness values are also reported and discussed.

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O28

THERMODYNAMICS OF AN Au-BASED GLASS-FORMING ALLOY

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Angell [1] has introduced the concept of melt fragility by analyzing the trend of liquid viscosity as a function of temperature. Later, he has termed thermodynamic fragility a parameter, m_T, in relation to the loss of entropy of the liquid phase on undercooling down to the glass transition temperature. The extensive thermodynamic quantities of the liquid are usually referred to the corresponding crystal and, therefore, depend on difference between the specific heat capacity of liquid and solid. As a consequence these quantities can be used to study the so-called melt fragility.

Although in recent years correlations between the kinetic and thermodynamic fragility indexes of various amorphous substances have been demonstrated, this is not yet proven for metallic glasses. Starting from a literature analysis, we review this topic and provide new experimental data on the specific heat capacity of an amorphous alloy, specifically $Au_{49}Cu_{26,9}Ag_{5,5}Pd_{2,3}Si_{16,3}$, the best Au-based glass-former. The specific heat capacity in the undercooled liquid, the amorphous phase and the crystal, and the heat of phase transformations were determined using a Diamond Perkin-Elmer DSC under high purity argon atmosphere. The differences in enthalpy, entropy were calculated, the m_T, parameter was derived and compared to both metallic and conventional glass-formers.

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O29

PERITECTIC MELTING OF ß-BORON IN B-C BINARY

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The melting behavior of ß-boron at the boron-rich side of the B-C binary phase diagram has long been an unsolved problem because of the difficulty of determining the small differences between the liquidus and solidus curves giving rise to speculations on either depleted, eutectic or peritectic reactions.

In order to define the reaction type, several floating zone crystal growth experiments on ßB(C) with varying amounts of carbon were quenched in order to analyse the chemical composition of the quenched molten zone and that of the zone-end part crystal corresponding to one set of data points on the liquidus and the solidus curve at the same temperature. A clearly peritectic melting behavior of ß-boron L+B_4C↔(ßB) was derived yielding a partition coefficient of carbon in ß-boron of about 3.

A thermodynamic modelling of the B-C system was performed via CALPHAD techniques incorporating the new data. The consequences of either a eutectic (L↔(ßB)+B_4C) or a peritectic reaction (L+B_4C↔(ßB)) on the liquidus in the systems M-B-C will be outlined for M=Ti, Zr, Hf, W.

O30

EXPERIMENTAL STUDY AND SIMULATION OF REVERSE SPINODAL DECOMPOSITION

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Long term aging of Fe-Cr alloys and steels leads to spinodal decomposition for typical temperatures in the range 250-400°C. Such a microstructure evolution has dramatic effects on structural martensitic steels as this increases their brittle to ductile transition temperature. In a preceding report [1] it was shown that differential thermal analysis (DTA) may be used for characterizing the extent of this evolution. For this, a DTA record is performed when heating the material from room temperature to a temperature at which it should be single phase. During this heating, a so-called reverse spinodal decomposition occurs that shows up in the DTA records. It was observed that the DTA signal is sensitive to the temperature at which aging had been performed as well as to the time of aging.

In order to better describe the changes occurring in the material during DTA runs, and thus for understanding the features shown by the DTA records, simulations have been performed using the approach recently developed by Jackson [2]. As the present work aims at understanding, a binary regular solution was adopted as in the original model. The only change made relates to the diffusion coefficient that depends here on temperature. The free energy G of the material was computed at each time step and the enthalpy was then calculated as $G - T\cdot\left(\partial G/\partial T\right)_p$.

The figure below shows the output of a 2D simulation, where the curve is the normalized enthalpy and the images illustrate the Cr distribution. An alloy with a composition C_0=0.2 was hold at T=0.45·T_C for 30000 step calculations, where T_C is the critical temperature, then heated at a rate of $2.10^{-4}\cdot(T/T_C)$ per step calculation. It is seen that the demixing was strongly marked at the end of the holding at T=0.45·T_C, very slightly changed at 0.6·T_C, starting to be smoothed at 0.75·T_C and nearly disappearing at T_C. At the end of the heating, at T=1.45·T_C, the material was totally homogenized.

The derivative of the enthalpy curve could then be compared to DTA records, and a series of calculations have been performed that illustrate the effect of temperature and time of aging.

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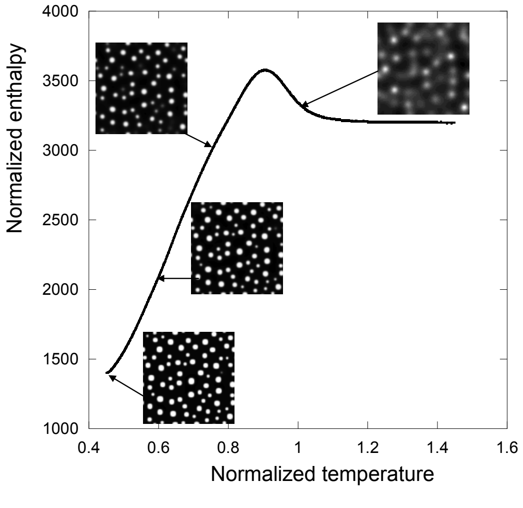

O31

THE USE OF PANDAT SOFTWARE IN THERMODYNAMIC CALCULATIONS RELATING TO LEAD-FREE SOLDER ALLOYS

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The value of *Computational Thermodynamics* to Materials Science is indisputable. Having the ability to make any number of complex calculations in respect to phase constitution with relative ease has provided a powerful tool in materials design and processing. A strong link to 'reality' is maintained owing to the underpinning of the technique with experimental observation.

Computational tools (software) have been around for a number of years now and undergo constant development. The *Pandat* software is a relative newcomer to the scene and has already made a reputation for itself owing to it's robust calculation engine and ease of use. Of course, it is not only the quality of the software that provides confidence in the calculations that can be performed by *Computational Thermodynamics* but also the quality of the thermodynamic databases that the software uses.

This presentation is essentially in two parts. Using the COST MP0602 thermodynamic database for High-temperature lead-free solders as an example, the methodology orf producing high-quality databases will be outlined. All calculations will be performed using the latest version of *Pandat* in order to show the capabilities of the software.

Acknowledgments: Grateful acknowledgement is extended to CompuTherm for the provision of the *Pandat* software and sponsorship of this presentation.

O32

THERMODYNAMICS OF THE FORMATION OF Zn-Al-Fe INTERMETALLIC COMPOUNDS IN MOLTEN ZINC BATH

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Keywords: Intermetallic compound; Hot-dip galvanizing; Supersaturation; Al-Depleted Zone

The shape, size, and composition of dross particles as a function of Al content at a fixed temperature were investigated for Al added to the premelted Zn-Fe melt simulating the hot-dip galvanizing bath by a sampling methodology. In the early stage less than 30 minutes after Al addition, local supersaturation and depletion of the Al content occurred simultaneously in the bath, resulting in the nucleation and growth of both $Fe_2Al_5Zn_x$ and $FeZn_{13}$. However, the Al was continuously homogenized as the reaction proceeded, and very fine and stable $FeZn_{10}Al_x$ formed after 30 minutes. An “Al-Depleted Zone (ADZ)” mechanism was newly proposed for the “$\eta \rightarrow \eta+\zeta \rightarrow \delta$” phase transformations. In the very early stage of dross formation, both Al-free large particles as well as high-Al tiny particles were formed. With a relatively high Al content, the nucleation of tiny η phase dross was significantly enhanced due to the high degree of supersaturation. This unstable η phase continuously dissolved and underwent simple transformation to the stable δ phase. The relationship between nucleation potential and supersaturation ratio of species is discussed based on the thermodynamics of classical nucleation theory.

O33

COHERENT AND INCOHERENT PHASE EQUILIBRIA OF BCC MISCIBILITY GAP IN THE Fe-Al SYSTEM

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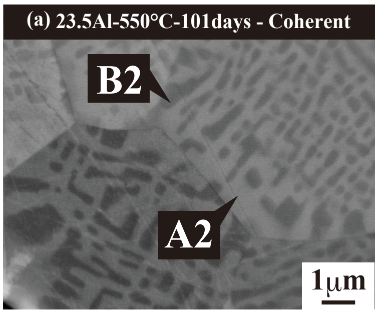
Allen and Cahn [1] suggested that the coherency of the equilibrium bcc phases, α(A2), α'(B2) and α"(D0$_3$), appeared in the Fe-Al binary system considerably affect the equilibrium composition and that discrepancies in equilibrium compositions reported by Okamoto *et al.* [2] and by Swann *et al.* [3] were caused due to the incoherent and coherent conditions, respectively. Ikeda *et al.* [4] also determined the equilibrium compositions of the miscibility gap at temperatures between 300 and 700°C using composition gradient samples, in which the coherency of microstructures were not taken into account. Recently, it was reported that the converge milling method, by which severe deformation can be introduced in powder samples, has some effects to obtain equilibrium microstructures at low temperatures below 600°C [5]. Making use of this technique, both coherent and incoherent microstructures could be formed and direct evidence of the effect of the coherency on the equilibrium compositions could be confirmed. In this study, the coherent and incoherent equilibria of the bcc miscibility gap in the Fe-Al binary system were investigated experimentally and thermodynamically.

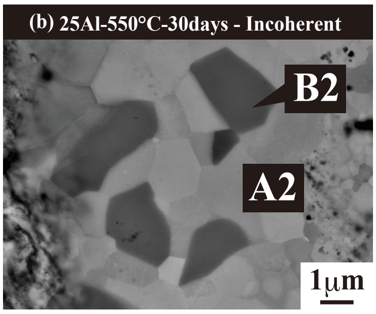
Gas-atomized powders of Fe-Al alloys were prepared. Coherent two-phase microstructures of the α(A2) + α'(B2) and the α(A2) + α"(D0$_3$) were obtained in the as-atomized powder by long-term heat-treatment at 550°C and 500°C, respectively. The spinodal decomposition occurred to form fine modulated microstructures, two phases of which were coarsened up to 1 μm in diameter by the Ostwald ripening during the heat-treatment as shown in Fig.1(a). To obtain incoherent microstructures, as-atomized powders were pre-heat-treated at 600°C, the condition of which are in α(A2) + α'(B2) two-phase region of the phase diagram in the Fe-Al system. After that, the powders were severely deformed by converge milling method. Then, each powder sample was encapsulated in an evacuated quarts capsule and equilibrated at temperatures between 400 and 600 °C for various durations up to 3 months. After that, each powder sample was molded in a conductive resin, mechanically polished, and finished by a vibratory polisher with 0.1 μm diamond suspension. Microstructure of cross section of the powder samples was examined and equilibrium compositions were determined by the FE-EPMA with low accelerating voltage of 6 kV.

Coherent and incoherent microstructures were shown in Fig.1(a) and (b), respectively. The recrystallization of the converge-milled powders resulted in the formation of equi-axed polycrystalline microstructure as shown in Fig.1(b). Results of FE-EPMA analysis were summarized in Fig.1(c), which confirms that the coherent equilibria shown with dashed curves appears inside of the incoherent equilibria shown with solid ones. According to the obtained phase diagram shown in Fig.1(c), the A2/B2 boundary shown with a hatched curve distorted towards Al-rich compositions below the crossing point with the Curie temperature curve, which suggests that the interaction effect between the chemical and magnetic orderings causes the anomalous distortion of the miscibility gap among the α(A2), α'(B2) and α"(D0$_3$) phases. Thermodynamic analyses of the coherent / incoherent equilibria and the interaction effect will be discussed.

(a) 23.5Al-550°C-101days - Coherent



(b) 25Al-550°C-30days - Incoherent



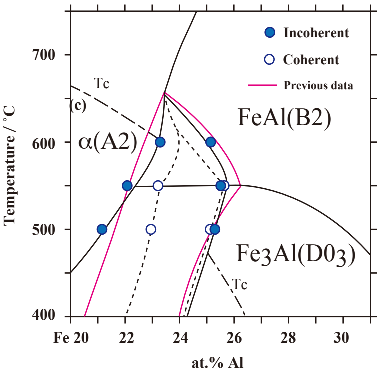


Fig.1 phase equilibria of BCC area in the Fe-Al system

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O34

EXPERIMENTAL STUDY OF THE Ta-Ge SYSTEM

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Keywords: Phase Diagram; Ta-Ge System; Germanides

The solid phases (Ta), αTa$_3$Ge, βTa$_3$Ge, αTa$_5$Ge$_3$, βTa$_5$Ge$_3$, TaGe$_2$ and (Ge) are known to be stable in the Ta-Ge system [1] but no information their equilibrium relations with the liquid was found in the literature. Therefore, the present work aimed at the experimental investigation of the phase diagram for this binary system. Samples were prepared by arc melting high purity Ta (min 99.8 wt%) and Ge (min 99.995 wt%) pieces under Ti-gettered Ar atmosphere. A sample with 95 at% Ge was melted by heating a mixture of βTa$_5$Ge$_3$ and Ge powders at 1100°C in an alumina crucible under Ar. The sample microstructures were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD). Samples containing 30 at% Ge were annealed between 1000°C and 1600°C in order to verify the $\alpha\leftrightarrow\beta$ transitions reported to occur for the Ta$_3$Ge and Ta$_5$Ge$_3$ compounds. All intermetallic phases, except for αTa$_5$Ge$_3$, were confirmed to be stable. Three eutectic reactions were observed with liquid compositions placed at 20.5; 28.0 and 97.0 at% Ge. βTa$_3$Ge and βTa$_5$Ge$_3$ solidify congruently while TaGe$_2$ is formed by a peritectic reaction. The eutectic decomposition L$\leftrightarrow$(Ta)+βTa$_3$Ge was measured at 2440±90°C by Pirani-Alterthum method. The absence of liquid formation during annealing show that the eutectic L$\leftrightarrow\beta$Ta$_3$Ge+βTa$_5$Ge$_3$ and peritectic L+βTa$_5$Ge$_3\leftrightarrow$TaGe$_2$ transformations occur above 2000°C. Further investigation is still necessary to confirm the αTa$_5$Ge$_3\leftrightarrow\beta$Ta$_5$Ge$_3$ transition in this binary system.

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O35

STRUCTURE AND DYNAMICS IN LIQUID SOLDERS: STRUCTURE FACTOR, DIFFUSION COEFFICIENTS, VISCOSITY AND ISOTHERMAL COMPRESSIBILITY

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Within the pseudopotential formalism, we developed a new model-pseudopotential able to describe accurately both heavy metals like tin and noble metals like copper and silver which are the basic elements of the new lead free solders. The pseudopotential describes the interaction between electrons and ions. The effective inter-ionic pair potential which takes into account the electron screening cloud, describes the atomic structure. It is deduced from the pseudopotential. It enters into a simulation program using Molecular Dynamics. A first result is the atomic structure factor that can be measured experimentally by neutron or X ray scattering. In the case of an alloy, partial structure factors describe the system. These can easily be calculated but in general cannot be obtained experimentally. Within the Bhatia Thornton structure factor formalism, it is possible to link the asymptotic behaviour of the structure factor to some thermodynamic properties like the isothermal compressibility. This has been done for pure elements. It is possible to follow the individual movement of particles and to obtain the different (self, hetero, inter...) diffusion coefficients. The collective movement of all particles can also be analysed by mean of the Green-Kubo theory to get the transport coefficients (shear viscosity). Diffusion coefficients are very difficult to measure accurately. Viscosity is a little easier to measure, but we observe high discrepancies between the different authors. It is thus important to be able to calculate accurately these properties by varying temperature and concentration for multi-component alloys.

O36

THERMODYNAMIC PROPERTIES OF LIQUID Ag-Sb-Sn ALLOYS DETERMINED FROM E.M.F. AND CALORIMETRIC MEASUREMENTS

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Keywords: Thermodynamics; Ternary system; Silver alloys; Enthalpy of mixing; Galvanic cell

The thermodynamic properties of the liquid ternary Ag-Sb-Sn system were determined with the electromotive force (e.m.f.) method using a galvanic cell with solid YSZ (yttria-zirconia) electrolyte:

Pt, Ni+NiO | YSZ | Ag-Sb-Sn+SnO2, Kanthal+Re

Three different cross-sections with constant Ag:Sb ratios of 3:1, 1:1 and 1:3 were applied to measure the thermodynamic properties of the ternary system in the temperature range between the liquidus temperature of the alloys and 1223 K. The partial free energies of Sn in liquid Ag-Sb-Sn alloys were obtained from e.m.f. data.

Additionally, the present work refers to high-temperature drop calorimetric measurements on liquid Ag-Sb-Sn alloys. The partial and integral enthalpies of mixing of liquid Ag-Sb-Sn solutions were determined along the following cross-sections of ternary system: $X_{Ag}/X_{Sb} = 1:1$ at temperature 1075 K and $X_{Sb}/X_{Sn} = 1:1$ at two different temperatures 912 K and 1075 K.

For the $X_{Sb}/X_{Sn} = 1:1$ cross-section the ternary system shows the S-shape change of the enthalpy of mixing versus X_{Ag} concentration. It changes from an endothermic enthalpy with maximum of approx. 110 J/mol to an exothermic minimum of approx. -3100 J/mol at XAg = 0.74. It implies the Ag-Sb-Sn system is characterized by the considerable change of ternary interactions from repulsive to attracting depending on the Ag concentration however, no significant temperature dependence was found experimentally. Generally, our measured values fit very well to most of the earlier reported results.

Obtained e.m.f. and calorimetric experimental data were adopted to calculate ternary interaction parameters of liquid Ag-Sb-Sn solution by applying the Redlich-Kister-Muggianu model for substitutional solutions. A full set of model parameters describing the concentration dependence of the tin activity and enthalpy of mixing was derived. From these data, the isoenthalpy and isoactivity curves were constructed at different temperatures.

O37

THERMODYNAMIC OPTIMIZATION OF THE V-Si-B SYSTEM

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In this work the thermodynamic modelling of the vanadium–silicon-boron ternary system was carried out using the CALculation of PHAse Diagram method. Data from the literature were used for the description of the binary systems [1-3]. In the case of the V-B system, new Gibbs Energy coefficients were established to comply with the experimental data from [4, 5]. Data from the isothermal section at 1600°C [6] and for the liquidus projection from Lima et al. [7] were used for the optimization of the ternary system. In order to describe the ternary system, two additional phases were included, T2 and D88, both modeled as solutions. The calculations based on the thermodynamic modelling are in good agreement with the experimental data available in the literature.

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O38

EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC MODELING OF THE MULTICOMPONENT Mg ALLOYS

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A thermodynamic database for multicomponent Mg alloys has been established using CALPHAD method, supplemented with key experiments and first-principles calculations. A series of experimental procedures have been designed to determine phase equilibria of Mg alloys. The pure element powders (or pieces) were mixed and pressed into pellets and then sealed into the Ta tubes using arc welding. These procedures were performed in a glove box to prevent the contamination and oxidation. The encapsulated samples were sintered at high temperatures, depending on the melting points of the alloys, and then annealed at 400 or 500ºC. Afterwards the samples were taken out from the Ta tubes in the glove box and analyzed using XRD, SEM and EPMA. The isothermal sections at 400 or 500ºC were established. In order to measure the invariant reactions and liquidus, self-made sealed Ta crucibles were used during DSC measurements. Using the presently obtained experimental data and first-principles calculated thermodynamic data, many systems were assessed for the first time and some systems were reassessed in order to have most up-to-date thermodynamic descriptions. Reliable thermodynamic descriptions of relevant systems available in the literature were incorporated into the database with necessary modifications to eliminate any inconsistencies. Key quaternary systems that contain the main components of important industrial magnesium alloys have been extrapolated to investigate the phase equilibria in these systems. Extensive calculations of solidification paths and phase equilibria have been performed for a number of multi-component industrial alloys, and compared with various experimental data such as phase fractions and phase transition temperatures. Good agreements between experimental data and calculations were obtained for many alloys, and are to be shown in this presentation.

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O39

THERMODYNAMIC PHASE EQUILIBRIA IN NIOBIUM SILICIDE-BASED ALLOYS

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Keywords: Nb-Si-Sn; CALPHAD; Phase diagrams; Refractory Metals; Silicides

Niobium silicide-based in-situ composites are potential candidate materials to replace nickel-based superalloys in the next generation of advanced gas turbines. These materials have excellent refractory and high temperature mechanical properties. To aid in alloy development and understanding of the properties of these alloys, a thermodynamic database is being developed using the CALPHAD method. Current systems of interest include Nb-Si-Ti-M and Nb-Si-Cr-M where M may be Sn, Hf, and Al etc. The addition of these elements is important as they can improve high temperature oxidation resistance, which for these alloys can often be poor.

Small additions of Sn (< 5at%) have been shown to significantly improve the oxidation properties, particularly within the pesting region (700-900°C) [1]. To understand the effect of Sn on equilibrium phases, a thermodynamic description is being developed. Recently a description based on limited available data [2,3,4] was published [5]. In order to better model this system, the ternary phase diagram has been reassessed based on new experimental data (phase analysis (XRD,SEM), thermal analysis (DSC/Cp)). Experiments were conducted to establish the stability range of Nb_5SiSn_2 and obtain thermodynamic measurements (e.g. Cp) to enable better parameter fitting. This assessment will be presented and compared to data from the literature.

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O40

THERMODYNAMIC ASSESSMENT OF Cr-Nb-C AND Mn-Nb-C SYSTEMS

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Keywords: Carbides; Thermodynamic assessment; *ab-initio* calculations

Niobium, manganese and chromium are common alloying elements for different types of steels. Precipitation of carbides in austenite leads to grain refinement and/ or strengthening of microalloyed steels. Cr-Nb-C and Mn-Nb-C systems are playing an essential role in studying carbide formation and accurate thermodynamic descriptions are important for further modelling-based approaches.

Despite wide usage of the mentioned above carbides in different combinations, there is an essential lack of experimental data describing interactions of carbides between each other. In the present work, an attempt to provide thermodynamic descriptions for the Cr-Nb-C and Mn-Nb-C systems, based on existing experimental data, extrapolations from binary systems and ab – initio calculations, was made. Various descriptions for most of the binary systems had been already available, so a selection between parameters sets was made. An additional reassessment was needed for the Cr-C system for the better suit with recent experimental data.

Existing experimental data on the Cr-Nb-C system provides us information about liquidus and solidus surfaces as well as several vertical sections. These data were used for the optimisation of the system. There is lack of experimental data on the Mn-Nb-C system. The existing experimental data mostly provides data on solubility products in steels. For this reason, the Mn-Nb-C system was assessed as an extrapolation from binary systems taking into account available experimental data from quaternary system Fe-Mn-Nb-C in combination with ab-initio calculations.

O41

EXPERIMENTAL INVESTIGATION OF THE R-Ni (R = RARE EARTH) SYSTEMS: ENTHALPY OF FORMATION OF THE RNi_2 PHASES

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The discovery of potential application in various fields of metal alloys containing both rare earths (R) and transition metals (T) has meant that during the past 50 years the study of their properties has received much attention. The increasing interest in the R-Ni systems and their alloys is related to the wide range of interesting technological applications. These alloys are generally recognized as members of the hydrogen absorption alloy family [1-2] and are currently used in battery productions. Thermodynamic and thermochemical data can be very useful for alloying design and processing. As far as enthalpies of formation are concerned, some data are available for different R-Ni system, especially in the Ni-rich region. Moreover, literature data are often contradictory and unreliable.

This study was designed to experimentally determine the standard enthalpy of formation of R-Ni (R=Nd, Sm, Gd, Tb, Dy, and Ho) alloys, especially for the RNi_2 composition.

A high temperature drop calorimeter [3, 4] has been employed to directly measure the heat of formation of the alloys at 300K. The calorimetric results have been validated by means of several analytical techniques. The state and composition of the synthesized samples have been checked by X-ray Powder Diffraction (XRD), Light Optical Microscopy (LOM), and Scanning Electron Microscopy (SEM). A high exothermicity in the formation of the RNi_2 phases has been observed, and the experimental results will be discussed and compared with literature data.

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O42

THERMODYNAMIC STUDY OF U – Si – C SYSTEM: SILICON ACTIVITY MEASUREMENTS AND THERMODYNAMIC MODELING

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The mixed carbide (U,Pu)C is the reference material for the fuel kernel of the Gas Cooled Fast Reactors for Generation IV future systems and silicon carbide, the reference material for the matrix. Chemical compatibility at high temperature between the kernel and the cladding was studied. In this framework, a thermodynamic database was developed on the U-Pu-Si-C system using the CALPHAD (CALculation of PHAse Diagram) to calculate phase diagram and thermodynamic properties. The experimental knowledge on the ternary U-Si-C is scare and uncertain and there is no thermodynamic properties for the liquid phase.

To improve the modeling of this system, we have measured the silicon thermodynamic activity for different compositions by multiple Knudsen cells mass spectrometry. Some solidus temperatures were also deduced. After each investigation, the samples were characterized using scanning electronic microscopy and X-ray diffraction. These experimental data were taken into account in the thermodynamic modeling.

O43

PHASE RELATIONS IN THE ZrO_2-La_2O_3-Y_2O_3-Al_2O_3 SYSTEM: EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC MODELLING

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Phase relations thermodynamic parameters of the ZrO_2-La_2O_3-Y_2O_3-Al_2O_3 system are important for development of new materials for thermal barrier coatings (TBC) and other applications like solid oxide fuel cell (SOFC) or nuclear materials. The La_2O_3-Y_2O_3-Al_2O_3 is a part of this system.

Phase relations in the La_2O_3-Y_2O_3-Al_2O_3 system were experimentally investigated. Samples were synthesized by co-precipitation method and heat treated at 1250, 1400 and 1600 °C. They were characterized by XRD and SEM/EDX. The results of experiments are in a good agreement with calculations based on binary extrapolation into a ternary system. Melting relations in the La_2O_3-Y_2O_3-Al_2O_3 system were investigated by DTA. Temperature and composition of eutectic reaction in the Al_2O_3-rich corner was determined by DTA followed by SEM/EDX investigation. The obtained results were used for assessment of ternary parameter in liquid phase. Thermodynamic database of the La_2O_3-Y_2O_3-Al_2O_3 system has been developed and phase diagrams are calculated.

The thermodynamic parameters of the La_2O_3-Y_2O_3 system were re-assessed using new calorimetric data for the $LaYO_3$ phase [1]. The obtained description was introduced into already available description of the ZrO_2-La_2O_3-Y_2O_3 system and parameters were adjusted for better fit to experimental data [2].

The derived thermodynamic database was combined with already available descriptions of ternary systems [3] to develop thermodynamic database of the ZrO_2-La_2O_3-Y_2O_3-Al_2O_3 system.

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O44-COSTMP0903

THE NANO-CALPHAD CONCEPT

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Keywords: Nano thermodynamics; Nano-Calphad

The abbreviation „nano-Calphad" stands for "Calculation of Phase Diagrams for nano-systems". The essential part of nano-Calphad is to introduce correctly the surface term into the equation for the Gibbs energy. In view of the controversy between the Kelvin and Gibbs equations, even this task has not an obvious solution (in the present talk the Gibbs method is preferred). However, there are many further questions to be addressed when the Calphad method is converted into the nano-Calphad method. This talk attempts to give the full list of all those problems, such as: i. the definition of a new, independent thermodynamic variable, ii. The extended phase rule, iii. the size dependence of the interfacial energies, iv. the dependence of interfacial energies on the separation between interfaces, v. the role of the shapes and relative arrangement of phases, vi. the role of the substrate (if such exist), vii. the role of segregation, taking into account its effect on the mass balance within multi-component nano-phases. It is also shown that the well known meaning of the tie line in binary two-phase fields is lost in nano-systems. The issues related to the size limits of materials thermodynamics and the need for a more complete databanks on molar volumes and interfacial energies are discussed.

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O45-COSTMP0903

PHASE STABILITY OF SMALL METALLIC PARTICLES: EXPERIMENTS AND CALPHAD THEORIES

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Small metallic particles on nanometer scale show unique size-dependent properties. The phase stability of metallic particles has attracted many attentions due to the promising applications in catalysis, nanoelectronics, etc. During the last decade, many experimental and theoretical studies have been carried out to investigate the phase stability of the small metallic particles on nanometer scale [1-9]. As an extension of the conventional thermodynamic expressions of bulk materials, Nano Calphad concept is considered as a useful tool to predict the phase stability of small particles. From the thermodynamic point of view, the size effect on the chemical potential can be described as a function of the particle size, the surface tension and the molar volume. Therefore, more reliable temperature dependences of the surface tension and molar volume are required. Recently, a new experimental system for electrostatic levitation (ESL) and thermochemistry measuremtns has been made in KRISS, Korea. With the help of ESL facility, the information of the surface tension and molar volume over wide temperature range including supercooled liquid region can be obtained. In this presentation, our recent progress in experimental and theoretical studies on the phase stability of small metallic particles on nanometer scale will be reported. And the potential of the ESL measurements in Nano Calphad will be suggested.

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O46-COSTMP0903

THERMODYNAMIC CALCULATION OF PHASE DIAGRAMS OF NANOALLOYS

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Surface energy of nanoparticles of alloys (nanoalloys) represents positive contribution to the Gibbs energy of individual phases which influences phase equilibria in respective systems. Surface energy is incorporated in the CALPHAD method into the expression for Gibbs energy of phases and phase diagram can be calculated.

In the presentation, calculation of phase diagram of system with complete miscibility of components in solid phases (Cu-Ni) will be shown and compared with the calculation for the system with partial miscibility of components in presented phases (Ag-Sn, Ag-Cu).

Verification of calculated phase diagrams is performed by chemical synthesis of nanoparticles of mentioned systems, their characterization by TEM and HRTEM and determination of phase transformation of nanoalloys by DSC.

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O47-COSTMP0903

BIMETALLIC NANOPARTICLE MODELING: TOWARDS NANOALLOYS PHASE DIAGRAMS

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Alloys phase diagrams are essential in the characterization of the equilibrium structure of the bulk alloys at finite temperature. The structural and chemical ordering has been the subject of intensive studies for a long time, notably from a theoretical point of view [1] and especially on metallic systems.

Surface segregation phenomena modify the chemical order inducing a competition or synergy between the surface segregation and the bulk ordering or demixing tendency, giving rise to an important investigation field from alloy surfaces to surface alloys [2].

More recently, nanoparticles have attracted much attention because of their wide variety of structure and morphology. Associated to chemical ordering and surface segregation in case of alloys, nanoalloys lead to complex systems [3]. The characterization of their equilibrium properties in their fundamental state (OK) and at finite temperature is of great importance in order to make the link between their structure and their properties.

We propose a theoretical study of the atomic structure, morphology and order/disorder transition versus surface segregation by Monte Carlo simulations using tight binding models of bimetallic nanoparticles with the tendency to ordering in the bulk alloy. Our theoretical results will be compared to experimental ones [4].

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O48-COSTMP0903

THERMODYNAMICAL ASPECTS OF PHASE SEPARATION TRANSITIONS IN BINARY AND TERNARY NANOALLOYS

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Keywords: Nanoalloys; Phase separation; Thermodynamic properties

We employed our recently introduced CBEV/FCEM method [1,2] in computations of the compositional-structure temperature dependence of equilibrated Pt-Ir and Pd-Ir cuboctahedron nanoparticles (NPs). For low Pt content, the occurrence of several smoothly varying atomic exchange processes between surface sites, which are reflected as distinct Schottky-type peaks in the configurational heat-capacity curve, are predicted [3]. Furthermore, 561- and 923-atom NPs of high-Pt content undergo ***intra-core*** separation-like phase transitions, reflected in abrupt changes in energy and entropy. The Pt inner core of the Pt-Ir NPs with onion-like structure at low temperatures, transforms into near-surface Pt-rich small clusters [3], while NPs having Ir-core and Pd-shell transform into solid-solution-like “phase”. Reduced size of the inner-core destabilizes it and results in lower temperature (and sharper) transitions. In addition, convexities in the low-temperature mixing free-energy curves indicate a tendency for ***inter-particle*** separation into Pd-Ir NPs having different overall compositions. The convexity disappears at a critical temperature signifying transition to a uniform system of solid-solution like NPs. The relationship between the two types of separation transitions as well as the role played by preferential strengthening of elemental surface-subsurface bonds are elucidated. The results furnish partial phase diagrams for the two binary NP alloys, and are compared with the macroscopic alloy miscibility gaps as well as with phase separation transitions predicted for the first time for ternary nanoalloys (Pt-Pd-Ir).

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O49-COSTMP0903

RELATIONSHIPS BETWEEN ALLOY AND NANOALLOY PHASE DIAGRAMS - AN ATOMISTIC VIEW

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Progress is reported in atomistic simulations with semi-empirical potentials to investigate various aspects of equilibrium nanoalloy phase diagrams and phase transformations, with a special emphasis on the relation with bulk phase diagrams.

Systems which do not mix in the bulk do not mix at the nanoscale either and are known to form nanoparticles with Janus-like or core-shell configurations. The situation is more subtle for systems with limited miscibility. Using the Au-Pt system as a case study, an embedded atom potential is parameterized so as to match the phase diagram exactly. As a specificity of the nanoscale, a smooth temperature dependence of the short range order parameter is found, which correlates with an onion-like configuration intermediate between solid solution and phase separated states.

Nanoalloys with high miscibility and cubic structure display the same ordered phases as their bulk counterpart. The role of thermodynamic driving forces and of mechanical stress in ordering is discussed using both four-fold and five-fold symmetrical Au-Pd systems as a case study.

The martensitic transformation known to occur in Fe-Ni alloys is found to correlate with a change of morphology in nanoparticles.

The effect of confinement on nanoalloy phase stability is considered. The example of Au-Pd is used to show that the effect of confinement on nanoalloys phase stability could be considerable. Encapsulation in carbon nanotubes represents a milder condition. Nevertheless, ordering of encapsulated Au-Pd clusters and wires appears to result from a competition between thermodynamic driving forces including the weak binding (van der Waals) to the nanotube. Encapsulated ordered Fe-Ni systems are not as sensitive to Van der Waals interactions but the confinement subsequent to the stiffness of the nanotube may affect the FCC/BCC transition in nanowires considerably.

POSTER SESSIONS

P1

EXPERIMENTAL INVESTIGATIONS OF THE STABILITY OF THE HIGHER MANGANESE SILICIDES

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Keywords: Higher Manganese Silicide; Phase diagram; Phase stability

The Higher Manganese Silicides (HMS), commonly referred to as $MnSi_x$ (x=1.72-1.75), are among the most promising semiconductors suitable for applications in thermoelectric energy harvesting systems, novel optoelectronic and photovoltaic devices. According to the Mn-Si phase diagram, the HMS belongs to the homogeneity range of the highest silicon-rich intermediate phase [1]. However, contrasting with this description, four different HMS phases, namely Mn_4Si_7, $Mn_{11}Si_{19}$, $Mn_{15}Si_{26}$, and $Mn_{27}Si_{47}$ are described in literature. Since they all possess a tetragonal unit cell with high anisotropy, the '*a*' lattice parameter being the same for all the structures and the '*c*' one being different, it is hard to distinguish these phases from one another by XRD [2-3]. This difficulty may explain why the stability range of the HMS has never been studied so far.

The aims of our work were to find a way to differentiate the HMS phases, then to investigate their stability domain both in composition and temperature, and finally to disentangle the antagonist descriptions previously mentioned.

Several alloys in the composition range 62-66 at. % Si, were prepared from their constitutive elements by arc-melting. The alloys were characterized by in-situ X-Ray Diffraction (XRD) measurements, Differential Thermal Analyses (DTA) and Electron Probe Micro Analyses (EPMA).

In this presentation, we will describe the method we used to discriminate the HMS phases in XRD patterns; we will give the set of results obtained from the experimental investigations and we will suggest some arguments as to why two antagonist descriptions were reported in literature.

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P2

STUDY OF SILVER CLUSTER FORMATION FROM THIN FILMS ON INERT SURFACE

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Keywords:Metal cluster;Tthin film; Melting; Silver; Coalescence

Nowadays a special attention of researchers is given to metal clusters formation because of their using in nanotechnologies. One of method of clusters formation is a thin film disintegration. In this connection we studied silver thin film evolution during heating in vacuum in dependence on film thickness in range from 6 to 130 nm.

An attention is given to factors determining clusters sizes during film disintegration. Investigation of clusters size distribution showed that two preferable clusters sizes is observed for (20-130)-nm-thick films after annealing at 660-800 ^{0}C. First preferable size corresponds to the diameter value 40-80 nm, second size is ~400 nm. For 6-nm-thick film clusters massive formed at 230 ^{0}C having one preferable size ~10-20 nm.

For (20-130)-nm-thick films annealed at 660-800 ^{0}C a visible evolution of clusters massive is observed in dependence on annealing duration, while for 6-nm-thick film annealed at 230 ^{0}C clusters massive was stable long time.

Evaporation and coalescence are reason for existence of two preferable cluster sizes in the case of 20-130 nm films: small-sized clusters are monoclusters consisting of unique nanocrystal and large-sized clusters are globular consisting of nanocryctals association. Since the disintegration temperature for 6-nm-thick film is low (230 ^{0}C), mentioned processes are not visible. As a result monoclusters are formed only. Correlations between clusters parameters, technology process parameters and original film thickness were revealed. Analytical form of mono- and global clusters distribution has been offered.

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P3

THERMODYNAMIC STUDY OF THE TERNARY B-Ni-X SYSTEM (X = Ti, Zr, Hf)

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Keywords: Phase diagrams; CALPHAD; Wetting; Joining; Borides

Diborides of elements belonging to the group 4 are characterized by outstanding properties, such as high hardness and thermal shock resistance; they belong to the class of Ultra High Temperature Ceramics (UHTCs) and play a key role in applications where stability to extremely high temperatures and damage tolerance are required. As they still pose problems of joining with themselves and with the underlying supporting structure, wettability of diborides by metals and alloys is thoroughly studied. In particular, the search for Ni-base brazing alloys has been undertaken [1], with the aim to design tough and durable joints.

Experimental findings deriving from sessile drop tests can be interpreted and supported from the basic point of view by multi-component phase diagrams calculated by the CALPHAD method [2,3,4]. For this reason, B-Ni-*X* ternary phase diagrams have been computed, basing on the available literature data and on the results of DTA analyses performed on Ni/ZrB_2 and on Ni-Zr alloys/ZrB_2 mixtures. The so obtained data could be used to explain experimental evidences and to predict the behaviour of systems not yet investigated experimentally.

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P4

THE ASSESSMENT OF PHASE EQUILIBRIA IN V-Cr-Si SYSTEM

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Keywords: Vanadium alloys; Silicide coatings; CALPHAD method; V-Cr-Si system

Considered as one potential candidate for core components of some generation IV nuclear systems, vanadium base alloys could be used as fuel cladding in Gas Fast Reactor (GFR) and also Sodium Fast Reactor (SFR). Vanadium is a semi refractory metal, having suitable mechanical properties under irradiation at high temperature [1], high mechanical formability as compared to the main other candidates such a SiC/SiC or ODS steels. However, vanadium is a trap to oxygen and its oxidation leads to the formation of non-protective oxide layer and oxygen diffusion in depth, also under low partial pressure of O_2 [2]. A new protective silicide coating, based on V_XSi_Y layers was developed by using the halide activated pack cementation (HAPC) process [3]. The successive coating layers obtained are consistent with the silicide series, as described in the binary phase diagram V-Si [4]. Further improvement of the oxidation resistance of coating could be obtained substituting V for Cr in V_XSi_Y layers. The knowledge of the thermodynamic data of V-Cr-Si system should allow choosing the optimised master alloy compositions leading to the optimised coatings, modified by Cr.

In the present work, the results of the thermodynamic assessment of the V-Cr-Si isothermal section are reported. Selected compositions of ternary alloys were prepared using arc melting furnace. Then samples were placed in sealed quartz tube under secondary vacuum and heat treated at 1200°C during 500 h. The phase equilibria were experimentally characterised using SEM, X-ray diffraction and electron probe microanalysis. A new ternary phase $(V,Cr)_{11}Si_8$ isostructural with $(Nb,Cr)_{11}Ge_8$ was detected.

Then, the isothermal section at 1200°C was calculated according to the CALPHAD method and compared to experimental data. Furthermore, the liquidus surface projection was constructed and calculated for this system using experimental data from as cast arc melted compositions. Seven Primary crystallization field Si, MSi_2, MSi, M_6Si_5, M5Si3, M_3Si and (V, Cr, Si) were identified.

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P5

STABILITY OF TERNARY COMPOUNDS WITH THE Fe_2P-TYPE STRUCTURE

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Keywords: Fe_2P-type structure; Ternary compounds; *Ab-initio*; Formation enthalpies

In the present paper, we performed first-principles calculations [1] of lattice parameters and enthalpies of formation of ternary compounds with the Fe_2P type structure (hP9, $P\bar{6}2m$, N°189) [2]. In this structure, the Fe atoms occupy the 3f (x_1, 0, 0) and 3g (x_2, 0, ½) Wyckoff positions and the P atoms the positions 1b (0, 0, ½), and 2c (1/3, 2/3, 0). Several ternary compounds crystallize in this structure: Ni_6Si_2B [2], Ti_6Si_2B [3], Ti_6Ge_2B [4], $T_6T'M_2$ where T is an early transition metal Zr or Hf, T' a late transition metal (Fe, Co, Ni) and M a p element (Al, Ga, Sn, As, Sb, Bi, Te) [2]. The ab-initio calculations allow to obtain the enthalpies of formation of these compounds. The calculated lattice parameters and internal parameters are in good agreement with the experimental determinations.

A large number of equiatomic ternary compounds of two transition metals and a p element crystallize also in the ternary-Fe_2P type structure. The prototype indicated in the Pearson Handbook [1] is ZrNiAl. In the case of the ternary Zr-Ti-Si system, we have shown that a compound with the Fe_2P-type structure is stable: TiZrSi. The Ti and Zr atoms occupy the 3f and 3g positions respectively while the Si atoms occupy the 1b and 2c positions.

For each compound the electronic densities of state have been computed. Both electronic and size effects allow to explain the stability of the ternary compounds.

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P6

THERMODYNAMIC MODELLING OF THE Fe-Nb SYSTEM

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Keywords: Fe-Nb system; Thermodynamic Modeling; CALPHAD

In this work the site occupancy and the enthalpy of formation of Fe-Nb intermetallic phases (Fe_2Nb and Fe_7Nb_6) were experimentally determined. For the site occupancy study, high purity Fe and Nb pieces were melted in arc furnace under argon atmosphere. Then, the samples were heat-treated in quartz tube, under vacuum, at 1150°C/700h and characterized by X-Ray Diffraction (XRD). The site occupancy was determined by Rietveld refinement of the XRD data. For the enthalpy of formation measurement, powders of high purity Fe and Nb (~325 MESH) were mixed in the intermetallic phases composition (33 and 48 %at. Nb respectively) and cold pressed. Then, the measure was made by direct reaction drop calorimetry at 1500°C. The results of this analysis and phase equilibria information from the literature [1] led to a CALPHAD modeling of Fe-Nb system.

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P7

ENTALL - THERMODYNAMICS DATABASE OF ALLOYS FOR SAFE HYDROGEN STORAGE AND ENERGY

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The Li-Si, Ag-Ca, B-Li, Ca-Li, and Al-Li alloys belong to the group of materials which have an applicable character. However, there is no available literature calorimetric data for these systems. With the use of the solution calorimetric method, the energetic effect of solutions of Li and the $Li_{22}Si_5$, $Li_{13}Si_4$, Li_7Si_3 and $Li_{12}Si_7$ intermetallic compounds in the acetic acid were measured and next the formation enthalpies of the compounds were calculated. The intermetallic compounds were prepared by means of melting lithium and silicon in a glove-box under the protective atmosphere of high purity argon. The obtained compounds were X-ray analyzed in order to confirm theirs structure. The TEM analysis of the precipitate obtained after the dissolution of the phases in the acetic acid showed that it was pure silicon. The measured heat of the reaction of Li in the acetic acid equals -261.1 ±1.6 kJ/mole and this value was applied in the calculations. As the silicon did not react with the acetic acid, the heat effect of the reaction was assumed to be zero. The values obtained for the formation enthalpy of the compounds are as follows: -24.4 ±1.7 for $Li_{22}Si_5$, -30.4 ±0.8 for $Li_{13}Si_4$, -29.4 ±1.0 for Li_7Si_3 and -25.6 ±1.9 for $Li_{12}Si_7$. "Iuventus Plus" project makes possible to create a new database of thermodynamics properties of alloys from Li-Si, Ag-Ca, B-Li, Ca-Li, and Al-Li systems. Entall database will contain the experimental data of formation enthalpy of intermetallic phases from these systems and software which allows to calculate other thermodynamic functions.

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P8

CALORIMETRIC INVESTIGATION OF RARE EARTH-MAGNESIUM ALLOYS

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Magnesium alloys are widely used in modern industry; their high strength properties combined with quite low density make them very attractive as structural materials in applications such as automotive and aerospace industry, industrial machinery etc. Commercially used Mg alloys are generally multi-component systems: detailed knowledge of the phase diagrams and thermodynamic properties of these complex systems and of their binary and ternary subsystems is very important for the development and design of new materials. Among the different elements employed as additives to magnesium-based alloys, an important role is played by the rare-earth (R) metals; their addition to Mg-rich alloys improves mechanical properties, such as ductility, high-temperature and corrosion resistance characteristics [1].

The thermodynamic properties of the compounds formed by magnesium alloyed with rare earths have mainly been investigated by vapour pressure measurements of magnesium over a series of two-phase alloys using Knudsen effusion techniques [2,3]. The enthalpies of formation of selected R-Mg alloys have also been obtained by solution calorimetry using acid aqueous solution or magnesium baths [4,5]. However, there appear to be serious discrepancies between the different values obtained for the enthalpies of formation and the thermodynamic properties of these alloys.

In this contribution experimental results on thermodynamic properties for different R-Mg alloys will be presented, discussed and compared with the data available in literature.

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P9

A PRELIMINARY ASSESSMENT OF THE Nb – Ni – Si SYSTEM USING AB-INITIO DATA

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Keywords: CALPHAD; Heat resisting alloys; Stainless Steels; Ab-initio calculations

The Nb – Ni – Si system may be considered a prototype for the development of cast superalloys for use in carburizing atmospheres, as the ones found in the petrochemical industry. The system is also important in the context of the development of heat resisting stainless steels for similar applications. For instance, the so-called G-phase, with the approximate stoichiometry $Nb_6Ni_{16}Si_7$, is found after heat treatment in 20%Cr, 25%Ni stainless steels stabilized with Nb [1] and in Nb-modified HK and HP centrifugally cast heat resisting tubes, where the G-phase precipitates seem to be somehow associated with the NbC particles in the eutectic with the γ phase [2]. The precipitation of the G-phase is suspected to be responsible for a dramatic reduction of ductility observed in these alloys after long-term service at temperatures around 700°C [2,3]. The only experimental information concerning this system, to the knowledge of the authors, is limited however to a 800°C isothermal section, published by Gladyshevskii et al. [3], and no thermodynamic assessment of this system has been published to date. The present work reports a preliminary assessment of the system based on ab-initio data. The heats of formation and bulk moduli of the compounds reported by Gladishevskii et al. [3] were determined using the FP-LAPW method, within the GGA approximation, as embodied in the Wien2K package. These results were then used to build thermodynamic models for the ternary phases and the silicon excess parameters for the μ-Ni_6Nb_7 phase. All compounds were modelled as stoichiometric compounds, except of the μ and the ternary C14 (Laves) phases, which were modelled as line compounds. Comparison between experimental and calculated isothermal section at 800°C shows a good agreement.

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P10

CRYSTAL STRUCTURES, PHASE RELATIONS, PHYSICAL PROPERTIES AND DFT CALCULATIONS IN THE Ge-RICH PART OF THE Ba-Rh-Ge SYSTEM

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Keywords: Phase relations; Crystal structure; Physical properties

The investigation of the Ge-rich (> 60 at%) part in the Ba-Rh-Ge system revealed the formation of three different ternary compounds at 750°C, the clathrate-I $Ba_8Rh_xGe_{46-x-y}\square_y$ with x_{max}= 1.2 crystallising in the cubic K_4Ge_{23-x} structure type, $Ba_6Rh_8Ge_{32}$ crystallising in an own structure type in the tetragonal space group I4/*mmm* with a = 0.65643 and c = 2.20367 nm, which is partially built up by $BaAl_4$-blocks, and $Ba_5Rh_{15}Ge_{36}$ crystallising in a remarkably large orthorhombic unit cell (space group: F*ddd* and a = 0.84750, b = 1.47250, c = 6.64450 nm), respectively. Phase relations were established at 750°C and 700°C by x-ray powder diffraction, electron probe micro analysis, and differential thermal analysis, revealing a decomposition of the clathrate-I phase below 740°C. Density functional theoretical calculations were applied in order to compare the stabilisation effect of Rh-incorporation into the clathrate framework with other transition metals. Physical properties of the new compounds, namely the electrical resistivity and the Seebeck coefficient were investigated.

P11

THERMAL ANALYSIS OF THE Ag-Bi-Cu SYSTEM

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Keywords: Ag-Bi-Cu; DSC

The Ag-Bi-Cu system belongs to a group of ternary alloy systems that until now are not fully studied. The literature survey indicated that the experimental data on this system are scarce. In particular, Zanicchi et al. [1] reported the existence of ternary eutectic at 240 ± 5 ^{o}C near Bi-rich corner without specifying the phases in equilibrium. Liu and Sun [2] on the other hand, based on a DTA study of 12 cross-sections, established ternary eutectic 258 ^{o}C at $Ag_{5.0}Bi_{94.5}Cu_{0.5}$ (at.%) and proposed the liquidus projection. In order to explain the differences and to provide reliable experimental data the DSC method was employed to study phase transitions with temperature in Ag-Bi-Cu alloys. The measurements were performed on samples of constant silver to bismuth mole fraction ratio 4:1, 1:1, 1:4, respectively, and varying copper content. The results obtained are discussed with the available experimental data and phase transition temperatures calculated based on the data of binaries from COST 531 thermodynamic database.

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P12

MODELING OF VISCOSITY OF BINARY ALLOYS FOR SURDAT-DATABASE. COMPARATIVE STUDY

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Comparative analysis between experimental and calculated values of viscosity was conducted. The calculations of viscosity were performed using Moelwyn-Hughes [1], Sichen - Boygen-Seetharaman [2], Seetharaman-Sichen [3], Kozlov-Romanow-Pietrov [4], Iida-Ueda-Morita [5], Kaptay [6], and Kucharski [7] models. In consequence, new equation was proposed for the viscosity modeling. Recalculated viscosities for many binary alloys shown better agreement with experimental data than those calculated from cited above the others models.

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P13

MODELLING OF OXYGEN TRANSPORT APPLIED TO Si-Ge LIQUID SYSTEM

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The growth of electronics industry has been accelerating as a result of progress in the semiconductor industry and improvement of semiconductor devices. $Si_{1-x}Ge_x$ mixed crystals possess electrical properties which offer distinct advantages over pure silicon for certain applications: high-speed electronic devices, thermoelectric converters, X-ray and neutron optics, and solar cells.

The key technology driving this progress involves crystal growth technique having high reliability. The crystal growth technique is strongly affected by the melt flow caused by variations in density, heat and mass transport phenomena, surface tension but also by its derivative with respect to temperature (Marangoni effect).

When investigating the surface tension, it is very important to take into account that many impurities can be surface-active, such as oxygen. The presence of oxygen at the molten metal interface and the existence of oxygen fluxes, from/towards the atmosphere yielding adsorption/desorption mechanisms, have the main effect in determining Marangoni flows, which rank among the main factors controlling the performance of such processes.

Theoretical models, relating the mass exchange between liquid metal systems and the surrounding atmosphere at different oxygen partial pressures, have been developed, which make possible an estimation of the degree of contamination of the surface and an explanation of the mechanism of the oxygen mass transfer at the liquid metal/gas interface.

An analysis of oxygen transport at the liquid metal surface of Si-Ge system is presented and compared with the available literature data.

P14

THERMODYNAMIC STUDY THE Ni-Pd-Te SYSTEM

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Palladium platinoid metal (Pd) and tellurium chalcogen element (Te) are fission products (FP) currently involved in the chemical processes of the nuclear fuel cycle, from the fuel life in the reactor to the waste management processes. In the binary systems, these metals both strongly interact with nickel (Ni) to form a Pd-Ni solid solution or Ni-Te intermetallic compounds.

In order to predict the high temperature interaction between these fission products and some nickel based structural materials, the Ni-Pd-Te ternary system was investigated. The thermodynamic description includes some experimental work (DTA + Analyses) and the modelling of this ternary system using the Calphad method. The experiments were supplemented by Scanning Electronic Microscopy coupled with EDS and WDS and by X Ray Diffraction of the samples to identify the phases. The observed microstructures and measured compositions are used to highlight the compositions of these FP metallic phases.

The Ni-Te binary sub-system was optimized using the available experimental data of the literature. For both Pd-Te and Pd-Ni systems, thermodynamic assessments were already available. Then, these binary descriptions were gathered and the contributions of two NiPdTe and $NiPd_2Te_2$ intermetallic phases were added to obtain the thermodynamic description of the ternary system.

This obtained database is used to calculate the Ni-Pd-Te phase diagram and some thermodynamic properties in order to predict the formation temperatures of (i) the eutectics and (ii) the intermetallic phases at high temperatures.

P15

THE Al-Ge-Ni PHASE DIAGRAM

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Superalloys for high temperature applications are very important materials in aircraft, space vehicle engines and turbines. Nickel or chromium are the basis for such superalloys, whereas the Nickel based superalloys are secondary hardened by addition of aluminium and hence the formation of the phase γ'-$AlNi_3$. Successful application of such materials requires effective joining technologies such as diffusion brazing. Therefore brazing materials with a lower melting point, but similar structural properties than the substrate are necessary. As germanium forms deep eutectics with aluminium and nickel, it is a possible candidate for brazing applications. The current work was performed with the aim to investigate phase equilibria and crystal structures in the Al-Ge-Ni alloy system, in order to optimise the composition of the brazing material and to better understand the interface reactions during the brazing process.

The ternary phase diagram was analysed using powder X-ray diffraction (XRD), light optical microscopy (LOM), scanning electron microscopy (SEM) in combination with energy dispersive X-ray spectroscopy (EDX), electron probe microanalysis (EPMA) and differential thermal analyses (DTA).

Two partial isothermal sections at 400 °C and 550 °C as well as a complete isothermal section at 700 °C were investigated experimentally. Furthermore vertical sections at 10, 20, 35, 55, 60, 70, 75 and 85 at.% Ni and at constant Al:Ni ratio of 1:3 were determined. Five new ternary phases were found to exist in the phase diagram. Four of them were structurally characterised, $\tau1$ ($Al_xGe_{2-x}Ni$, Ge_2Ni-type), $\tau2$ ($Al_{67.5}Ge_{18.0}Ni_{14.5}$, own type), $\tau3$ ($Al_yGe_{9-y}Ni_{13\pm x}$, $Ga_3Ge_6Ni_{13}$-type) and $\tau4$ ($Al_xGe_{2-x}Ni$, CaF_2-type), while the last one, $\tau5$, is probably a superstructure of the B8-type, which was not yet solved.

Moreover a liquidus surface projection and a reaction scheme of the system were determined. Altogether, 17 invariant phase reactions, including 1 degenerated eutectic, 6 peritectic reactions, 7 transition reactions, 1 maximum and 2 yet not clearly referable reactions were discovered.

P16

THERMOPHYSICAL PROPERTIES AND WETTING BEHAVIOUR OF SnSb-BASED ALLOYS

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Sn-Sb alloys with good electrical characteristics relevant to soldering and different melting temperatures make a base for lead-free solders as a substitute for the lead-rich Pb-Sn high-temperature solders. The available experimental data on the SnSb-based alloys are rather limited and scattered.

In this contribution we report the thermophysical properties and wetting behaviour of the SnSb-based alloys with additions of Cu and Bi. The melting and solidification temperatures as well as the respective enthalpies have been determined with the differential scanning calorimetry. The mass density, surface tension, and contact angle on copper substrates have been investigated by the sessile drop technique. The effects of the substrate surface quality and the rest air pressure in the experimental chamber on the wetting have been studied.

P17

THE 4th LAW OF THERMODYNAMICS

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Keywords: CALPHAD; Solution thermodynamics; Laws of nature; European paradox

The rule of Lupis and Elliott (LE rule) proposed for the first time in 1966 is reformulated in this talk as: ‘Real solid, liquid and gaseous solutions (and pure gases) gradually approach the state of an ideal solution (perfect gas) as temperature increases at any fixed pressure and composition’. This rule is rationalized through heat expansion of phases and loss of any interaction with increased separation between the atoms. It is shown that the rule is valid only if the standard state is properly selected, i.e. if mixing does not involve any further hidden phase changes, such as melting. It is shown that the necessary and sufficient practical conditions to obey the LE rule is the equality of signs of the heat of mixing and excess entropy of mixing and the non-equality of signs of heat of mixing and excess heat capacity of mixing of the same solution. It is shown that these two conditions are fulfilled for the majority of experimentally measured high temperature solutions. The LE rule is compared to the existing laws of thermodynamics. It is shown that the LE rule can be considered as a potential 4th law of materials thermodynamics.

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P18

INTERFACE INTERACTION AND WETTING IN THE Ta_2O_5/Cu-Me (Me = Al, Ti) SYSTEMS

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Keywords: Tantalum pentoxide; Metal melts; Interaction; Wetting, Thermodynamic evaluation

Tantalum pentoxide (Ta_2O_5) displays transparency in a wide wavelength range, low losses and high stability in the near UV and IR regions and has very high reflection index. Due to these advantages it is extensively used in the electro-optic devices. One of the drawbacks of Ta_2O_5 is its moderate thermodynamic stability and enhanced reactivity with metals and oxides, which complicate Ta_2O_5 soldering to other materials. In this study the interface interactions and wetting behavior in the Ta_2O_5/Cu-Me (Me=Al, Ti) systems were examined. The contact angle for Ta_2O_5/Cu system is about 100deg. at 1533 K, while the alloying of Cu with Al or Ti lead to an improved wetting. Nevertheless, the effect of these active elements on the contact angle is different. In the Ta_2O_5/Cu-Al system contact angle decreases gradually with increasing Al content down to 47deg. for pure Al, while in the Ta_2O_5/Cu-Ti system, addition of even 13at%Ti leads to significantly lower contact angle (< 20 deg.). SEM and EDS analysis indicate that at the Ta_2O_5/Cu-Ti interface two layers are formed: a continuous (~ 10 μm thickness) TiO_2 layer attached to the drop and a layer which consists of a TiO_2 and Ta_2O_5 mixture (15μm) attached to the substrate. For the Ta_2O_5/Cu-Al interface thin (1μm) alumina layer attached to the drop was observed an beneath it the presence of relatively thick $AlTaO_4$ layer (30 μm) was detected. We suggest that wetting improvement is attributed to the nature of the reaction product formed at the interface. Moreover, the morphology of the interfacial layers was explained using thermodynamic properties of the Ta-Cu-Al , Ta-Cu-Ti and Ta-Ti-O, Ta-Al-O systems.

P19

THE ELECTRONIC PART OF MELTING ENTROPY AND ELECTRONIC STATES SPECTRUM IN SEMICONDUCTOR MELTS

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A new method to estimate electronic part of melting entropy for semiconductors with degenerated electronic gas has been established. Obtained relations give a possibility to estimate electronic part of melting entropy only on the base of experimental data on electro-physical and magnetic properties of substances in solid and liquid states. These relations demonstrate well the change of chemical bonding type at melting. The relation between electronic part of melting entropy (ΔS^{el}) with melts' electronic spectrum factor (or Mott factor g) has been found. There was also shown, that the value of electronic part of melting entropy determines charge transfer mechanism in explored systems. This is due to the fact that ΔS^{el} value is related to the melt metallization degree because of the free electrons' concentration increase during melting.

P20

ABOUT CHANGE OF EFFECTIVE MASS OF STATES' DENSITY AND ELECTRONS MOBILITY AT THE MELTING OF METALIZING SEMICONDUCTORS

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On the basis of the knowledge on electronic part of melting entropy, there was proposed a new method to estimate the effective mass of conducting electrons (m_n^*) in the semiconductors melts. On the example of the $A^{III}Sb$ compounds there is shown that melting according to the type semiconductor – metal is accompanied by a sharp increase of the m_n^* value. This suggests huge changes in energy spectrum of charge carriers at the phase transitions of this type. The electron mobilities u_n in liquid and solid phases at the melting temperature were also calculated. The sharp drop of the charge carriers' mobility at melting was shown. We have noticed a correlation in variations of m_n^* and u_n at phase transition and concluded that such situation is typical for substances which melt according to the type semiconductor – metal.

P21

THERMODYNAMIC ASPECTS OF HIGH TEMPERATURE OXIDATION ON A 304 STAINLESS STEEL

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The nature and the stability of the surface oxides formed during high temperature oxidation of stainless steels are key information in order to optimize their removal at the end of the production process. Nonetheless, the oxidation is a complex phenomenon [1], driven by both thermodynamic and kinetic parameters. So, a comparison of experimental data and theoretical calculations could give new insights on process modelling.

In this study, the high temperature oxidation of a 304 stainless steel is studied, combining experimental and theoretical methods. Commercial samples have been taken at selected steps of the line production process. In addition, samples were oxidized under various N_2/O_2 atmospheres in the 800-1100 °C temperature range.

Oxides products have been investigated by Scanning Electron Microscopy (SEM) and X-ray diffraction (XRD). The structure, composition and relative amount of crystal phase were evaluated by means of Rietveld refinement of XRD data.

Thermodynamic functions for the temperature and composition dependence of the free energy of M_2O_3, M_3O_4 and MO (M=Fe,Cr,Ni,Mn) phases were collected from the literature [2]. A thermodynamic database has been implemented in the Thermocalc software in order to obtain thermodynamic information.

Oxides formed after annealing are strongly dependent on the processing parameters (i.e. annealing atmosphere, temperature gradient). Composition and relative amount of oxides obtained from experiments and calculations matches reasonably for annealing at high temperatures, but differs significantly at low temperatures. So, the oxide scale growth was followed via termogravimetric analysis and a kinetic models has been developed in the Dictra software.

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P22

EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC CALCULATION OF THE Au–Ga–Sb PHASE DIAGRAM

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Keywords: Au–Ga–Sb system; Phase diagram; Phase transformations

Phase diagram of the Au–Ga–Sb ternary system was extrapolated using calculation of phase diagrams (CALPHAD) method. The liquidus projection, invariant equilibria and six characteristic isopleths were calculated. In the experimental part of the work, phase transition temperatures of the selected samples with compositions along calculated isopleths: GaSb–AuGa$_2$, GaSb–AuGa, Au–GaSb, Sb–AuGa, GaSb–Au$_{0.3333}$Sb$_{0.6667}$ and Ga–Au$_{0.5}$Sb$_{0.5}$ were measured using differential scanning calorimetry (DSC). Experimentally determined phase transition temperatures were compared with the results of thermodynamic calculation. Also, predicted phase equilibria at room temperature were compared with the experimental data from the literature.

P23

BULK AND SURFACE THERMODYNAMICS OF MONOTECTIC LIQUID ALLOYS

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Keywords: Monotectic liquid alloys; Bulk thermodynamics; Surface tension; Interfacial energy; Surface phase transition

The following thermodynamic properties of monotectic alloys are treated together as function of temperature and composition:

- excess Gibbs energy of bulk liquid alloy, described in accordance with Gibbs and with the 4th law of thermodynamics [1],
- surface tension of the liquid alloy in accordance with the Butler equation, but using parameters being characteristic for the liquid (and not for the solid) alloys [2],
- the surface phase transition (SPT) line can be found in accordance with the prediction of Cahn and using the Butler equation [3-4],
- the liquid/liquid interfacial energy can be found using an extended Butler equation [5],
- the solid/liquid interfacial energy and the contact angle is found for non-reactive and not-dissolving solid substrates,
- the interfacial phase transition (IPT) line can be found at the liquid/solid interface.

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P24

PHASE TRANSFORMATIONS IN THE TERNARY Ag–Ga–Sb SYSTEM

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Keywords: Ag–Ga–Sb system; Phase diagram; Phase transformations

Phase diagram of the Ag–Ga–Sb ternary system was extrapolated using calculation of phase diagrams (CALPHAD) method. Phase transition temperatures of the alloys with compositions along three vertical sections with constant molar ratios Ga/Sb=1, Ag/Ga=1 and Ag/Sb=1 were measured using differential scanning calorimetry (DSC). Scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM/EDS) was used for identification of phases in equilibrated samples. Experimental results were compared with thermodynamic prediction.

P25

TRANSFORMATIONS IN LIQUID HYPO- AND EUTECTIC Pb-Bi ALLOYS

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Liquid hypo- and eutectic Pb–Bi alloys have been characterized from room temperature to 650 °C by Mechanical Spectroscopy (MS), i.e. damping and dynamic modulus measurements, and X-Ray Diffraction (XRD) at high temperature.

MS experiments have been carried out by using a new technique developed by us; it employs hollow reeds of austenitic stainless steel filled with the alloy to study and sealed at the extremities. The reeds are mounted in free-clamped mode in the sample holder and excited by a sinusoidal signal at the free end.

Melting of alloys is accompanied by Q^{-1} maxima corresponding to the critical points of phase transitions showed in the phase diagram for each composition. After completion of melting all the alloys exhibit a maximum (O) with a corresponding slight *E* slope variation; the intensity and position is different depending on alloy composition. Such behaviour can be explained by considering a transition from heterogeneous to homogeneous melts.

In addition, the eutectic alloy shows from 350 °C to 520 °C a remarkable modulus drop accompanied by a broad Q^{-1} maximum. In the same temperature range radial distribution functions (RDFs), determined from X-ray diffraction patterns, evidenced variations of the mean distance between the 1st nearest neighbour atoms. The anelastic phenomena have been attributed to a structural re-arrangement of liquid metal.

To clarify whether the original structure of liquid metal influences somehow the microstructure of the resulting solid, each alloy has been quenched by the liquid state both above and below the temperature of maximum O and examined by XRD. The results evidence different short-range ordering of the solid.

P26

INTERACTION OF OXYGEN IN TERNARY LIQUID Ag-X-O ALLOYS

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Keywords: Thermodynamics; Silver alloys; Galvanic cell; Dilute alloys; Oxygen interactions

The knowledge of oxygen interaction in dilute liquid alloys plays an important role in the technological processing of many metallic substances, mainly in thermodynamic description of metal-slag equilibrium as well as the phenomena at the solid metal/oxide interface. The main aim of present work is to develop data of the influence of selected second solute element X on the oxygen interaction in ternary silver alloys. The activity coefficients of oxygen, f_O, in dilute liquid alloys Ag-X-O (X = Pb, Sb, Se, Te) were determined by a coulometric titration method using solid oxide galvanic cell with the YSZ zirconia electrolyte:

Iridium; oxygen in Ag-X-O | O^{2-} | air; Platinum

in temperature range from 1285 K to 1485 K.

To compare the influence of solute elements the first order interaction parameters of oxygen in liquid silver alloys according to Wagner-Chipman method:

$$e_o^{Me} \equiv \lim_{x_{Ag} \to 1} \left(\frac{\partial \ln f_o^{Me}}{\partial x_{Me}} \right)_{P,T}$$

have been estimated as the functions of temperature.

At the end, the known literature data together with the present data of ln f_O as a function of X_X were collected and compared with one another at Kaldo process temperature 1373 K.

P27

CONTRIBUTION TO THE THERMODYNAMIC DESCRIPTION OF THE Bi_2O_3-Al_2O_3-PbO SYSTEM

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Keywords: Bi_2O_3-Al_2O_3-PbO system; Lead-bismuth eutectic; Phase diagrams; Calphad method; Spallation target

In the new generation reactor called Accelerator Driven System, a spallation target consisting of lead-bismuth eutectic liquid (LBE) is in direct contact with the spallation window made of T91 steel, causing damage to the window due to oxygen in LBE. An idea is to develop aluminium or chrome protective coatings for the T91 steel. In order to verify the efficiency of these coatings, a thermodynamic investigation of the complex system (Pb-Bi-Hg)-(Fe)-(Al-Cr)-O is necessary. The aim of the present work is to describe the sub-system Bi_2O_3-Al_2O_3-PbO according to the CALPHAD approach in order to enrich a database already initiated in our laboratory by Diop [1] and Michel [2] on Bi_2O_3-PbO and Al_2O_3-PbO respectively.

The system Bi_2O_3-Al_2O_3 had been investigated during many studies. Different versions of phase equilibria diagrams in air were suggested in literature. That is the reason why it was necessary to identify all different phases and invariant reactions of the system Bi_2O_3-Al_2O_3. Different compositions of mixtures of oxide powders were pressed into pellets and isothermally annealed at different temperatures during 1 to 8 weeks. After annealing the samples were quenched in water using a silica tube, then inspected using X-ray powder diffraction and SEM. Additional techniques like thermogravimetric analysis and solution calorimetry are planned. The same way was applied to the experimental investigation of the Bi_2O_3-Al_2O_3-PbO system.

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P28

THE RELATIONSHIP BETWEEN THE PHASE DIAGRAM, STRUCTURE AND THERMODYNAMIC PROPERTIES IN THE Ba – Ge SYSTEM

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Keywords: Phase diagram; Liquid state; Thermal effects; Clathrates

The construction of the Ba-Ge phase diagram based on the results of the differential thermal analysis is a serious problem because of the formation of the metastable phases in this system. Prokofieva V. together with her colleagues (Elektronik tekhnologia 3, 25 (1969); Izv. Akad. Nauk SSSR, Neorg. Mater. 6, 580 (1970)) have carried out the detailed study of the phase equilibria in the concentration interval 0 - 40 at.% Ba. Three clathrate compounds which belong to the various types of structures are formed around the eutectic point in this range of the diagram. The results of these works, obtained by means of the methods of physical and chemical analysis don't agree with those of the new data (W. Carrillo-Cabrera et al (2004, 2005); M. Pani and A.Palenzoni (2008)) regard to the nature of some phase transformation, composition and stability of clathrate compounds. It concerns the nature of melting for the Zintl phase $BaGe_2$ and thermal stability of the clathrate Ba_8Ge_{43}. In earlier studies, the additional thermal effects in the liquid and solid states were fixed whose nature is still unclear. Unfortunately, this is not discussed in the new papers. The typical features of clathrate compounds are known to be unusual structure and electronic properties. The short-range order based on the clathrate structure may exist even in the liquid state in the Ge-Ba system. Therefore metastable phases can be formed under non-equilibrium crystallization.

This paper is devoted to the thermodynamic analysis of phase diagram in the Ba-Ge system in the germanium-rich part with using the data on structural and thermophysical properties for the pure Ge and the Ba-Ge melts. The nature of thermal effects, the features of the temperature dependences for viscosity, conductivity and ultrasonic propagation velocity in the liquid state are discussed. Specific attention is paid to the analysis of temperature and concentration dependences of the volume properties of the melts. The inner pressures for liquid germanium and eutectic melt are compared. Thermal effects observed in the liquid phase are considered from the different points of view. Possible change nature of chemical bonds with temperature and the influence of charge transfer are analyzed.

P29

STABILITY OF LAVES PHASE IN THE V-Zr SYSTEM BELOW ROOM TEMPERATURE

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Keywords: Laves phases; Zero Kelvin; Heat Capacity; Einstein Temperature

The transformation from non-Laves phase to Laves phase at low temperature when the temperature is increased is well known [1]. This transformation from the rhombohedral ZrV_2 structure to the cubic C15 Laves phase occurs at about 110-115 K and its experimental data were described in details in [2,3].

A new analysis of this anomaly with the help of ab initio calculated total energies and phonon spectra is presented and its consequences for the phase diagram of the V-Zr system are discussed. For a proper description of the transformation from non-Laves phase to Laves phase, the extension of SGTE unary data to zero Kelvin temperature [4] was employed.

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P30

THERMOPHYSICAL PROPERTIES OF LIQUID Ga-In-Sn EUTECTIC ALLOY

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Keywords: Ga-In-Sn; Electrical conductivity; Thermoelectric power; Viscosity; Surface phenomena

Gallium forms alloys characterized by specific properties with the majority of metals and metalloids. Many of the Ga-based alloys are low-melting; the physical and mechanical properties of some metals are enhanced when seeded with gallium. Unlike many liquid metals, the Ga-In-Sn eutectics is chemically compatible with a wide variety of metals, plastics, rubbers, and glasses at low temperatures. The alloy also has more attractive cooling and handling properties than those of Hg, Pb, and Pb alloys. Ga-In-Sn and its variant alloys have potential uses in numerous applications.

It is commonly used as a mercury replacement in thermometers and tilt switches. The alloy is a working fluid for studies of bubble driven flows in industrial technologies and excellent medium for investigation of thermoelectromagnetic convection in a shallow square layer of liquid metal. Besides, this alloy shows considerable potential in liquid metal experimental research in general, mainly because of its beneficial properties and the fact that it is liquid at room temperature.

Discrepancies in the reported eutectic compositions and other physical parameters require new precise measurements in order to obtain reliable data on the main thermophysical properties over a wide temperature range.

In the present paper, measurements are reported on the electrical conductivity, thermoelectric power, viscosity, thermal conductivity, surface tension and density of the Ga-In-Sn eutectic in the temperature range between the melting temperature and 700 K. Related temperature correlation fits are derived and compared with those available in literature and could be recommended as input for thermodynamic simulations.

P31

HIGH TEMPERATURE LEAD-FREE SOLDERING: PHASE EQUILIBRIA OF (Cu,Ni)-Sn-Zn SYSTEM

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Keywords: Ternary alloy systems; Ternary intermetallics; Phase diagram; Crystallography; Lead-free solders

Lead has been prohibited by legislation for electronic and household applications due to environmental concerns and toxicity. Still a potential replacement is required for high temperature (260-350 °C) applications. Sn would serve a major role in the upcoming new HT lead-free soft solders due to its compound formation ability, low melting, ductility and cost effectiveness. Small additions of Ag, Cu or Ni leaded to suitable low-temperature solders which are already at the market, e.g. SAC-alloys. In order to enhance the melting regime of such solders Zn could be added. As Ni and Cu are frequently used as substrate materials which are involved in interfacial reactions with the solder, the system (Ni, Cu)-Sn-Zn is important for the design of new HT soft solders.

This study focuses on the experimental investigation of (Ni, Cu)-Sn-Zn system. Several isothermal sections have been established between 1100-500 °C for Ni-Sn-Zn and at 180 °C for Cu-Sn-Zn. At least six new ternary compounds have been identified using X-ray and metallographic methods, the structure of four of them could be already solved by single crystal XRD. Several isopleths and a liquidus projections could be evaluated which provide useful information for understanding and control the soldering process. Finally, a Scheil diagram, a liquidus projections as well as isotherms and isopleths based on the DTA, XRD and metallographic investigations will be shown

The Ni-Zn binary system has been newly investigated and shows only slight changes compared to the version compiled in Massalski's book[1]. The experimental from alloy samples have been supplemented applying isopiestic vapor pressure methods to determine activities, phase transformations and to prepare proper single crystals.

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PRESSURE DEPENDENCE OF THE PHASE EQUILIBRIA IN THE Sn-P SYSTEM

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The basics of soldering of Ni(P) substrates with Sn based solders has been a research topic within COST Action MP 0602. Naturally, the ternary Ni-P-Sn phase diagram (including the corresponding binary boundary systems) was a major issue since it will be necessary to understand the reactions occurring in the soldering process.

The most relevant literature information on the binary Sn-P phase diagram, as collected by Massalski et al. [1], dates from the first half of the 20th century [2]. It shows three intermetallic compounds (Sn_4P_3, Sn_3P_4, SnP_3) and two liquid miscibility gaps forming syntectic reactions with Sn_4P_3 and SnP_3. During an attempt to check the proposed phase equilibria it was discovered that traditional experimental methods failed for P contents of more than about 10 at% and that phase equilibria are strongly pressure dependent. Already earlier it had been found that the compound Sn_3P_4 is only stable for certain partial pressures of P [3].

Using a so-called isopiestic vapor pressure method in two variants, Sn samples were equilibrated with P vapor at a given pressure. This provided not only partial thermodynamic properties of P for binary Sn-P alloys but gave also information on the phase equilibria as a function of temperature and pressure. It was discovered that the "syntactic" reactions in Refs. [1, 2] are most probably peritectic type decomposition reactions, i.e. Sn_4P_3 = L + G and Sn_3P_4 = Sn_4P_3 + G. The variation of the different invariant reactions with pressure was derived for P contents of up to about 60 at%.

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P33

NUMERICAL PREDICTION OF THERMODYNAMIC PROPERTIES OF TERNARY ALLOYS

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This paper presents a new numerical approach to modeling of ternary systems on the basis of thermodynamic properties of binary systems included in the investigated ternary system. The Muggianu extension of the Redlich-Kister formalism is a widely accepted description of the excess Gibbs energy of ternary systems.

$$^{ex}G^{\phi} = \sum_{i\neq j}^{n} x_i x_j \sum_{z=0}^{m} {}^{z}L^{\phi}_{ij}(x_i - x_j)^z + \sum_{i\neq j\neq k}^{n} x_i x_j x_k L^{\phi}_{ijk}, \text{ z = 0,1,m.} \qquad (1)$$

where ${}^{z}L^{\phi}_{ij}$ are binary and, L^{ϕ}_{ijk} ternary temperature dependent interaction parameters optimized on the basis of the available thermodynamic and phase diagram data.

$$L^{\phi}_{ijk} = x_i\,{}^{0}Lx_{ijk} + x_j\,{}^{1}L^{\phi}_{ijk} + x_k\,{}^{2}L^{\phi}_{ijk}\,, \qquad (2)$$

Usually binary systems are well investigated, so ${}^{z}L^{\phi}_{ij}$ parameters are known, but not many ternary alloys have been investigated, so L^{ϕ}_{ijk} parameters for many systems are unknown. Unless the formula and ${}^{z}L^{\phi}_{ij}$ parameters are known, the idea of calculating L^{ϕ}_{ijk} parameters can be regarded as solving an Eq.(1), when all boundary conditions (for binary *ij* alloys) are known. The approach proposed in this paper is as follows: if we know all boundary conditions, that is ${}^{ex}G^{\phi}$ values on all legs of the Gibbs triangle we find a function value inside the triangle.

Results of calculations were compared with data for Cu-Sn-Zn and Bi-Cu-Ni systems obtained by means of the CALPHAD method.

P34

ALUMINIUM DIFFUSION IN ALUMINIDE COATINGS DEPOSITED BY THE CVD METHOD ON PURE NICKEL

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The diffusion behavior of Al in aluminide coatings formed by the CVD process was examined by the analysis of Al concentration against the distance in pure nickel specimens aluminized for various times (15 min, 1 hour, 4 hours and 8 hours) at 1273 and 1323 K. Coatings consisted of three layers. The β-NiAl phase was on the surface of the coatings, whereas γ-NiAl and γ'-Ni$_3$Al formed deeper parts of the coatings. Diffusion was calculated for each phase by the use of the finite differences method. In solving the equations, it was accepted , that for a c(x) function, it is possible to approximate its derivative (slope / tangent) at a certain point by: the slope of the arc described as the difference of functions at the end of the calculation area or by the slope of the arc described as a reverse difference of functions – close to the coating's surface; or by the slope of AB arc given as a central difference of functions – inside the sample.

P35

CALORIMETRIC STUDY OF SOME Bi-Cu-Sn ALLOYS

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The paper presents results of calorimetric investigation of the Bi-Cu-Sn system by means of differential scanning calorymetry DSC at the temperature interval 300-1500 K, values of the liquidus and solidus temperature, the melting enthalpy and heat capacities of the selected alloys. Some microstructure investigations of the alloys were performed by the use of a scanning electron microscope (SEM).

Heat capacity of the investigated alloys was described by the Kelley's equation presenting the temperature dependence of heat capacity at temperature above 0^0C. Values of Kelley's equation parameters were calculated on the basis of the experimental results for the temperature ranges between transformations. The Knopp-Neuman rule, that postulates the additivity of the heat capacities of the elements is obeyed in some temperature ranges.

The presented investigation is a contribution to an overall examination of the Cu-Ni-X-Y systems (X, Y = Sn, Bi, Zn, Ti) in relation to development of a new lead free solders in the frame of the Action COSTMP0602.

P36

THE Co-Ni-Ti ISOTHERMAL SECTION AT 900 °C

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The experimental investigation of the Co-Ni-Ti phase diagram is part of a larger project aimed at developing a thermodynamic database for the Co-Fe-Ni-Ti quaternary system. Co-Fe-Ni-Ti and its sub-systems are relevant to different materials: from Ni- and Co-based superalloys to hard magnetic materials, from Ti-based corrosion-resistant alloys to amorphous and metastable phases. Moreover, from a more fundamental point of view, they are an interesting example of systems where both structural and magnetic ordering occur and interact.

Co-Ni-Ti had been previously studied by several investigators using diffusion couples and equilibrated alloys. Several isothermal sections and a pseudobinary CoTi-NiTi section were established. The isothermal sections agree to each other in the Ti-richer part (at $x(\mathrm{Ti}) > 0.5$) but disagree at lower Ti content, especially about stability and phase relations of the Ti(Co,Ni)3 ternary phase.

Several samples have been prepared by arc melting small pieces of the component elements. After equilibration at 900 °C they have been characterised by optical and scanning electron microscopy, electron probe microanalysis and X-ray powder diffraction. As a result the 900°C isothermal phase diagram has been determined, with special attention to the low Ti region (at $x(\mathrm{Ti}) < 0.5$). In particular stability, crystal structure and phase relations of the Ti(Co,Ni)3 ternary phase have been confirmed and / or determined in the present investigation.

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THERMODYNAMIC AND PHYSICAL PROPERTIES OF LIQUID ALLOY IN TERMS OF FREE VOLUME THEORY

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Keywords: Free volume theory; Al-Zn; Sn-In

Nowadays, computer modelling is wide applied for the simulation of dependence of thermodynamic and physical properties on the composition of alloys. Most of such models aim at prediction of thermodynamic properties but only few focus on the simulation of physical properties. An important theory allowing to model both, physical and thermodynamic properties is the free volume theory [1]. In our research, we used it to create a reversible simulation path enabling to obtain the thermodynamic and physical data, simultaneously, under specific conditions. Our initial studies showed the importance of excess entropy for the development of an accurate and reversible simulation path. Therefore we focused on the improvement of a basic expression for excess entropy proposed by Tanaka and Gokcen [2]. This expression consists of two parts: configurational and vibrational, both describing atom in its nearest neighbours (*cell*). Our improvements addressed the second (vibrational) part.

Our model was tested for both kinds of non-ideal solutions, displaying positive and negative deviation from Roault's law (Al-Zn, Sn-In). The introduction of our corrections into the free volume model enabled to diminish divergence between modelled and experimental data. The modelled transport properties for liquid alloys are in high degree compatible with experiment, when such improvement is imposed. Obtained results were explained in terms of structural properties like concentration-concentration structure factor at the long wavelength limit ($S_{cc}(0)$) [3] and Warren-Cowley short range order parameter (α) [4,5].

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P38

IMPACT OF Ce ADDITION ON Cu-PHASES IN A380 ALLOY

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Keywords: A380 alloy; Cerium; Precipitation; Kinetics; Eutectic

The purpose was to establish the influence of Ce on precipitation kinetics of Al_2Cu phase and the formation of eutectic phase (α-Al + Al_2Cu) in A380 alloy. Thermal analysis and differential scanning calorimetry (DSC) were used to examine the influence of Ce on precipitation kinetics of Al_2Cu precipitate in A380 alloy. Furthermore, scanning electron microscopy (SEM) and focussed ion beam (FIB) were used to analyse modified morphology of eutectic phase (α-Al + Al_2Cu). The precipitation of Al_2Cu precipitates takes course more rapidly and intensively, therefore reaction kinetics is increased when Ce is added to the alloy. The appearance of eutectic Al_2Cu phase in Ce-modified A380 was more compact. Ce partly dissolved in Al_2Cu-eutectic phase which caused a coarser formation of Al_2Cu-phase.

P39

THE SYSTEMS TANTALUM (NIOBIUM) – COBALT – BORON

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Keywords: Phase equilibria; Liquidus surface; Crystal chemistry; Hardness

Constitution of the ternary systems Nb-Co-B and Ta-Co-B was studied, employing optical and electron microscopy, X-ray powder, single crystal diffraction, electron probe microanalysis, DTA and Pirani melting point measurements. Ternary phase equilibria were determined within an isothermal section at 1100°C. For the Co-rich part (≥50at%Co) of the system, a liquidus surface projection and a corresponding Schulz-Scheil reaction scheme were constructed. The crystal structures of novel ternary compounds have been elucidated by X-ray powder and single crystal diffraction and were supported by TEM. {Nb,Ta}CoB with NbCoB-type exhibits a high temperature modification (ZrAlNi-type), which was only present in as cast alloys, but found to be stabilized by the addition of Fe to annealing temperatures of 1400°C. $Ta_3Co_4B_7$ was proven to be isotypic with $Nb_3Co_4B_7$. Orthorhombic $\{Nb,Ta\}Co_2B_3$ represent novel structure types with branched boron zig zag chains. $\{Nb,Ta\}Co_2B$ was found to adopt a unique monoclinic structure type very close to an orthorhombic setting. Substitution of Co by Ni stabilizes a smaller orthorhombic lattice with Re_3B-type structure (Cmcm) although no homologue compound in the Ni-system exists. The crystallographic relations among the structure types of Re_3B and pseudo-orthorhombic as well as monoclinic $\{Nb,Ta\}Co_2B$ were defined in terms of a Bärnighausen scheme. DFT calculations revealed very close stabilities for the three competing structure types for $\{Nb,Ta\}Co_2B$. Detailed transmission electron microscopy for Nb(Co,Fe)B, $\{Nb,Ta\}Co_2B$, $\{Nb,Ta\}(Co,Ni)_2B$ and $Ta_3Co_4B_7$ confirmed lattice geometries and crystal symmetry. Vickers hardness was measured for $\{Nb,Ta\}Co_2B$, $\{Nb,Ta\}(Co,Ni)_2B$ and $\{Nb,Ta\}_{2-x}Co_{21+x}B_6$revealing the highest value of hardness of *HV*=17.6±0.9 GPa for $TaCo_2B$.

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AN ASSESSMENT OF THE Mg-Fe-Si SYSTEM

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Keywords: Mg-Fe-Si system; Thermodynamics

Mg alloys are attracting increasing attention as promising alternatives to Fe and Al alloys in an effort to reduce the weight of structural materials. A knowledge of the thermodynamics and phase equilibria of the Mg-Fe-Si system is critical for this application.

This ternary system has been assessed several times [1,2], where the thermodynamic description of Fe-Si sub-system has come from [3]. However, in this work an inverse miscibility gap in the liquid phase appears at around 2500 K. Because of this and the recent publication of new experimental data for that system, the Fe-Si system has been re-assessed. The liquid phase was described using a substitutional solution model without taking into account the associated species that have been reported in the literature. The order-disorder transformation of the BCC phase has been described using a single Gibbs energy function. The compound phases have been treated as stoichiometric as only small homogeneity ranges are observed experimentally.

No ternary compounds have been reported in the ternary Mg-Fe-Si system, and the solubility of third element in the binary compounds can be neglected. The ternary interaction parameters for the liquid and solid solutions have been optimized in this work. A consistent thermodynamic description of this ternary system has been produced using description of the Fe-Mg, Mg-Si and Fe-Si subsystems taken from [4], the COST 507 database and this work, respectively. Solidification paths for several key Mg-rich alloys have been simulated using the Scheil solidification model.

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P41

THERMODYNAMICS AND PHASE EQUILIBRIA OF Ga-Me (Me = Al, Au) ALLOYS

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Keywords: Thermodynamics; Ga alloys; Ga-Al; Ga-Au

The results of thermodynamic study and characterization of two binary Ga-based systems –Ga-Al and Ga-Au system, are presented in this paper. Calorimetric study was done using Oelsen methodology and partial and integral molar thermodynamic quantities were determined at different temperatures. Phase equilibria investigations were done experimentally - using differential thermal analysis, light optic microscopy and scanning electron microscopy with EDX, and analytically - using CALPHAD method. Obtained results agree well with available literature data.

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P42-COSTMP0903

SIZE DEPENDANCE OF THE CHEMICAL ORDERING OF Cu-Ag NANOPARTICLES

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Copper and silver are two elements which are immiscible in the bulk and which have been shown to form $\mathrm{Cu_{core}Ag_{shell}}$ structures in small clusters. We investigate how surface and interface energies of Cu-Ag systems depend on the thickness of each phase, aiming to model the core-shell to Janus transition which has been experimentally observed in Cu-Ag clusters for sizes larger than 10 nm. The structural transition of systems with this size is beyond the scope of direct computational approaches at the atomic level. Therefore, we extensively study surface and interface effects at the atomic level in order to understand the key factors governing the crossover between core-shell and Janus structures at larger sizes and to build a continuous model capable of predicting and characterising this transition. For this purpose we use an empirical Gupta potential to model the interatomic cohesion and we study systems with fcc crystal structure and with flat and spherical geometries. These results provide a basis to quantitatively characterise how the energy balance of a given nanoparticle geometry varies with nanoparticle size.

P43-COSTMP0903

STRUCTURE AND THERMODYNAMICS OF Ag-Cu NANOALLOYS: A COMPUTATIONAL STUDY

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The structure and thermodynamics of AgCu core-shell chiral clusters is investigated by global optimization searches and molecular-dynamics simulations. It is shown that, when size increases, the most stable core-shell icosahedral structures become chiral [1], because of a concerted rotation of the facets in the outer shell. This transformation to chiral structures is confirmed at the density-functional level, and it is rationalized in terms of simple bond-counting argument. It is also shown that the same transformation takes place in AgNi, AgCo and AuNi clusters, and that the chiral motifs is favourable in a wide size range around magic sizes [2]. The study of the thermodynamics focuses on the melting phase transition which is investigated by molecular-dynamics simulations. These simulations show that the chiral icosahedra melt in the same temperature range as pure icosahedral clusters of comparable size [2].

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P44-COSTMP0903

METAL NANOPARTICLES: SYNTHESIS, MORPHOLOGY AND THERMAL BEHAVIOUR

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In recent years, metallic nanoparticles (NPs) have gained much attention due to their applications as catalysts, in electronics, in electro-optics and for changes in surface plasma band energy [1,2].

Their shape, size, composition, crystalline nature and structure can be controlled by the experimental conditions during the production. Various synthesis techniques have been reported in literature (both physical and chemical methods and also a combination of them); the specific advantages of chemical reduction of metal ions with alkaline borohydride technique such as its simplicity, versatility and scalability to massive production have been underlined [2,3].

The experimental approach in our research has been to synthesize Ag, Cu and Ag-Cu eutectic nanoparticles by a low temperature chemical reduction method in aqueous solution adopting potassium or sodium borohydride as a reducing agent. X-ray powder diffraction (XRD) and Transmission Electron Microscopy (TEM) was used to determine the crystalline nature of the samples, the size and the composition of the particles. The thermal behaviour of the samples has been investigated by Differential Scanning Calorimetry (DSC).

TEM analysis showed particles with irregular shape due to their aggregation; the composition of the particles was measured by Energy Dispersive X-Ray Spectroscopy (EDX): Ag=80.2, Cu=19.8 at.%. XRD analysis confirmed the nanoparticle components. DSC measurements performed on heating reveal an endothermic peak at ~770°C that could be related to the binary (L $\leftrightarrow$ (Ag) + (Cu), T=780°C) eutectic reaction [4].

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P45-COSTMP0903

THE EFFECT OF THE PHASE SIZE AND SHAPE ON THE Ag-Cu (NANO)PHASE DIAGRAM

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Keywords: Nano-phase diagram; Ag-Cu; Shape effect; Size effect

In order to extend the CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) technique to nanosystems, the thermodynamic description involving the phase size and shape was employed in the calculation of the phase diagram of the Ag-Cu system [1]. Size and shape dependent contributions have been added to the system description and the chemical potentials and the excess of Gibbs energies were reassessed as a function of composition, temperature, phase size and shape factor.

Figure 1 shows the effect of the phase size on the Ag-Cu phase diagram on example of spherical particles with a diameter of 10 nm and 100 nm. A shift of the liquidus to lower temperatures is observed as the phase size is decreased. The eutectic temperature is lowered and the eutectic point composition is shifted to the silver side. The increase of the shape factor enlarges the effect of the phase size on the system.

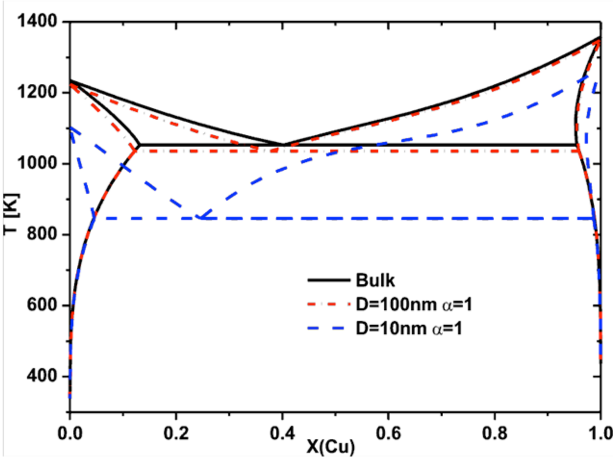

Figure 1: Phase diagrams of the Ag–Cu system calculated for different nanoparticles size

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P46-COSTMP0903

THE CALCULATION OF THE PHASE DIAGRAMS OF NANOALLOYS USING AB-INITIO SURFACE TENSION CALCULATIONS

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CALPHAD approach is a very useful technique for calculation of phase diagrams of bulk materials based on thermodynamic database containing data such as chemical potentials of pure substances and excess Gibbs energy of mixtures as a function of composition, temperature and pressure. When an attempt is made to use the CALPHAD approach to small particles on nano scale, the chemical potentials and the excess Gibbs energy are dependent on additional parameters: the particle size, and surface tension.

The ab-initio calculations are used to model theoretically the surface effects by means of surface energy and surface tension calculations. The phase diagram calculations were done for the Ni-Sn system, using ab-initio and experimental results for surface tension and the dependence of the phase diagram on particle size and crystallographic orientation of the nano-particle was also studied.

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P47-COSTMP0903

SYNTHESIS AND CHARACTERIZATION OF Sn-RICH Ni–Sb–Sn NANOSOLDERS

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Keywords: Thermodynamics; Ternary system; Silver alloys; Enthalpy of mixing; Galvanic cell

Nano-crystalline samples of pure Sn and of Sn-rich ternary Ni–Sb–Sn alloys, with compositions ranging from 80 to 97.5 at% Sn and a Ni to Sb molar ratio of 1:1, were synthesized by reduction of stoichiometric metal chloride solutions with $NaBH_4$ at 0°C in alkaline medium. The particle sizes of the obtained alloys, measured by TEM/SEM, were found to be in the range of 40–350 nm. A relative decrease in melting temperature of up to 15°C was observed for these alloys compared to a bulk sample. A sample with 95 at% Sn was subjected to heat treatment at 180°C for various time periods up to 5.0 h to study particles with well defined average sizes between 50 and 135 nm. The melting temperatures of the annealed samples were found to increase progressively with increasing particle size. At the same time, the excess surface energy of these heat treated samples was measured as a function of particle size using a Calvet type calorimeter. From the differences of the (H_{573}–H_{299}) values between nano and bulk samples, the excess enthalpies for nano-sized samples were derived to be between 18.8±1.9 and 0.8±1.4 kJ g^{-1} for particle sizes between 50 and 135 nm.

P48-COSTMP0903

ABOUT THE MODELLING OF THE SURFACE TENSION OF LIQUID Ag-Au ALLOYS

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Keywords: Ag-Au; Surface tension; Perfect solution; Butler model; QCA for the regular solutions; molecular dynamics simulations

The surface tension of liquid Ag-Au alloys has been calculated by different theoretical approaches. A lens type phase diagram of the Ag-Au system and a close similarity of its pure components in terms of the Hume-Rothery empirical factors (atomic radius, crystal structure, valence difference) indicate that so called perfect solution model, as the most simple one, could be used for the calculation of the surface tension. The other two macroscopic models available in the literature, i.e. a classic thermodynamic model based on the Butler equation and the Quasi-Chemical Approximation (QCA) for the regular solutions, developed in the framework of statistical mechanics combined with Quasi Lattice Theory (QLT) have been also used to calculate the surface tension isotherms of Ag-Au melts. Molecular dynamics simulations using an embedded-atom model potential and the mechanistic route were carried out to compute the pressure tensor and the surface tension of liquid Ag-Au alloys, thus aiming to bridge the gap between thermodynamic models for phase diagrams and atomistic simulation.

In addition, the surface effects on the microscopic functions are also discussed. The structural characteristics of Ag–Au melts are expressed in terms of the two microscopic functions, i.e. the concentration fluctuations in the long-wavelength limit and the Warren–Cowley short-range order parameter. The results obtained are compared among them as well as with the corresponding literature data. Some discrepancies between the experimental and theoretical data were found.

P49-COSTMP0903

UNRAVELLING THE SURFACE STRUCTURE OF PdGa INTERMETALLIC COMPOUND BY AB INITIO THERMODYNAMICS

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Pd-Ga intermetallic compounds (IMCs) have shown remarkable catalytic properties for an important reaction step in the polyethylene production, namely the semi-hydrogenation process of acetylene [1-3] to ethylene. However, the reaction pathway is largely unknown. To address this question we refer to model cases: PdGa single crystal surfaces. The bulk crystal and electronic structure of PdGa have been reported earlier [1-2,4-7] however, the geometry of stable surface terminations, determining the activity and selectivity of the catalyst, was still unknown.

Here we combine *ab-initio* thermodynamics, quantitative low energy electron diffraction (LEED-I(V)), high-resolution scanning tunneling microscopy (STM), to unequivocally identify the surface terminations of PdGa(111) and (-1-1-1) surfaces. Both surfaces exhibit significant differences in catalytic activity that are exemplified by calculations of hydrogen dissociation.

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P50-COSTMP0903

EXTENSION OF THERMODYNAMIC DATABASE FOR THE CALCULATION OF NANO-SIZED PHASE DIAGRAMS

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Keywords: Thermodynamic databases; Nano-sized phase diagrams; Surface tension

Thermodynamic databases have been used mainly for phase diagram calculation, but they can be also applied to the calculation of thermophysical properties, such as surface tension and viscosity. The CALPHAD (**Cal**culation of **Pha**se **D**iagrams) approach has been widely recognized in different fields of materials science and engineering[1, 2] and subsequently, the method has been successfully extended to the calculation of phase diagrams for nano-sized materials characterized by simple shape, such as “lens type” (complete solubility), eutectics and monotectics. In order to support the thermodynamic approach, that is according to[3] for particles up to at least up to 100 nm, the existing databases have to be extended in view of additional requirements in order to be useful for all classes of nanomaterials.

The thermodynamics of solid-liquid phase equilibria in small particle systems has been studied initially by analysing the melting phenomena of pure metals and alloys[4, 5]. It has been established that the melting points of some pure metals decrease with decreasing size of their metallic particles[6]. The large surface / volume ratio in nano-sized particle systems has significant effects on their thermodynamic properties and phase relations[7]. Simple phase diagrams of segregating binary nano-sized alloy systems, such as Cu-Pb, Au-Si, Ag-Cu[6,8,9] have been calculated successfully as a function of temperature (T), composition (c), size (d) and taking into account that the phase relations are dependent upon the size of particle and its surface property. The surface tension of small particles may change owing to curvature, which may decrease with decreasing size, yielding the liquidus temperature drop[10].

In order to support the assessment of nano-sized phase diagrams, an extension of thermodynamic databases is required. The new databases should contain data on the interfacial tensions, i.e. surface tension of liquids and solids as well as the data on the depression of melting temperature of metals and alloys related to a decrease in particle size. In the framework of the COST 531, the database SURDAT, containing surface tension data of lead-free solders, has been developed to aid in new solder design and also giving the possibility of being combined with thermodynamic databases to assess phase diagrams for nano-sized materials. Similar initiatives have been undertaken in the framework of COST Action MP0602, and the data collected can also be transformed into a similar database.

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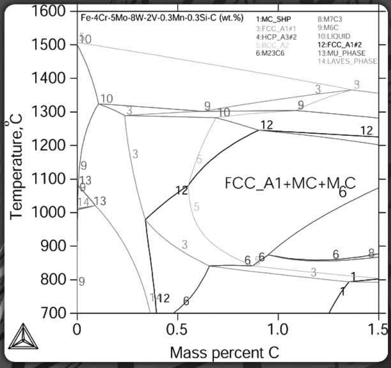
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3:FCC_A1#1
4:HCP_A3#2
5:BCC_A2
6:M23C6
8:M7C3
9:M6C
10:LIQUID
12:FCC_A1#2
13:MU_PHASE
14:LAVES_PHASE
FCC_A1+MC+M6C
Temperature, °C
Mass percent C
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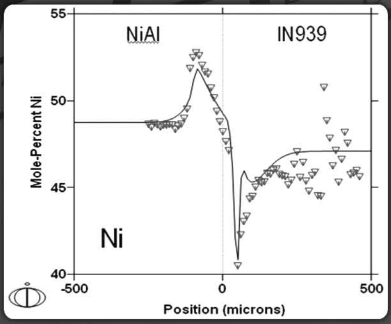
1500
1400
1300
1200
1100
1000
900
800
700
0
0.5
1.0
1.5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Position (microns)
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50
45
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0
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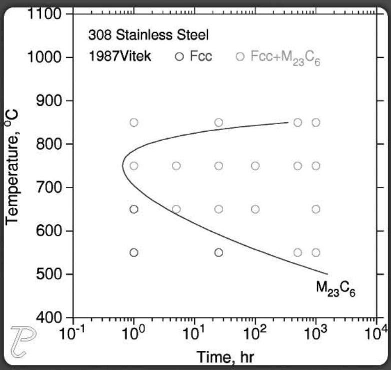
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Fcc
Fcc+M23C6
M23C6
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Time, hr
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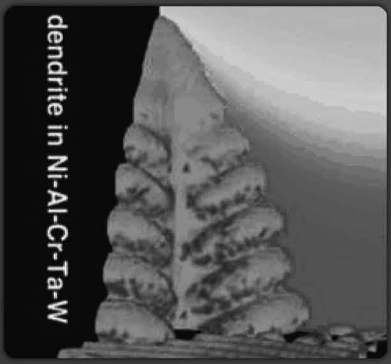
dendrite in Ni-Al-Cr-Ta-W