PROGRAMME

TOFA 2022

**18th Discussion Meeting
on Thermodynamics of Alloys**

THERMODYNAMICS OF ALLOYS

SEPTEMBER 12–16, 2022

KRAKOW

September 12–16, 2022, Kraków, Poland

This book contains the abstracts submitted by the participants for the 18th Discussion Meeting on Thermodynamics of Alloys TOFA 2022.

The professional quality of the abstracts is the authors' responsibility.

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TOFA 2022

September 12–16, 2022

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WELCOME NOTE

Dear Colleagues and Friends,

Welcome to the 18th Discussion Meeting on Thermodynamics of Alloys (TOFA 2022). It is the second time that TOFA is held in Krakow after the meeting in 2008. This year, our TOFA 2022 will be held live, with only few presenters joining our meeting remotely. The number of participants is similar to the last meeting in Bad Staffelstein, Germany in 2020, but lower than it used to be in the past. Still, we have a four-day program full of interesting presentations.

TOFA 2022 follows a well established tradition of a single-session conference with selected oral presentations and a poster session, with plenty of time and op-portunities for discussions and networking. Nearly a third of this year's meeting participants could be described as early stage researchers. The TOFA confer-ence continues to be a place where early stage researchers and experienced colleagues, both experimentalists and theoreticians, scientists focused on basic research and those focused on application related topics come together.

Exceptionally this year TOFA 2022 will be held in parallel to the 10th Inter-national Conference on High Temperature Capillarity. The oral sessions will be held separately but social activities will be shared, giving both communities an opportunity to meet.

Looking forward to an excellent meeting.

Przemyslaw Fima
Meeting Chair of the TOFA 2022

GENERAL INFORMATION

VENUE
NOVOTEL KRAKOW CITY WEST
11 Armii Krajowej Street, 30-150 Kraków, Poland

DATE
September 12–16, 2022

SCIENTIFIC ORGANISER
Dr Przemyslaw Fima
Institute of Metallurgy and Materials Science, Kraków, Poland

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Philip Nash (USA)
Rada Novakovic (Italy)
Raymundo Arroyave (USA)
Simona Delsante (Italy)
Suzana G. Fries (Germany)
Tetsuo Mohri (Japan)
Toshihiro Tanaka (Japan)
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Yong Du (China)

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ŻYDEK Arkadiusz

GENERAL INFORMATION

INFORMATION FOR PRESENTERS

Please prepare your presentations as PDF or Power Point in 16:9 aspect ratio. Please upload your presentation well ahead of time of your presentation.
Note the allotted presentation time (presentation + discussion time):
Invited talks   30–35 min presentation + 5–10 min discussion
Session talks   15 min presentation + 5 min discussion

POSTER SESSION

Authors are requested to be present at their posters during the poster session. Poster boards will be numbered. You will find your poster number in the book of abstracts. Please note that all posters should be hanging in the designated area on Tuesday, 13 September, by 16:00.

SOCIAL PROGRAMME

Get together, Monday, 12 September
Take a part in Get together on Monday, 12 September, 18:00 at the conference venue.
Guided tour of Krakow's Old Town and conference dinner, Wednesday, 14 September
The tour starts at 15:50, from the conference venue the busses take us near the Old Town. After the guided city tour we meet at 19:00, at Conference dinner, at restaurant "Szara Kazimierz", ul. Szeroka 39, Kraków. There will be no organized transportation from the restaurant to the conference venue after the dinner.

CONFERENCE FEES

Conference registration fees include:
– Access to all Conference Scientific Sessions
– Conference Proceedings
– Coffee breaks as in the final program
– Lunches as in the final program
– Get together reception
– Conference dinner
– Excursion

Accompanying person fees include:
– Get together reception
– Conference dinner
– Excursion

SCIENTIFIC PROGRAMME

17:00–20:00   Registration
18:00–18:20   Opening
18:30–20:00   Get together

Tuesday, 13 September 2022

9:00–9:20   Opening address

Session 1
Chair: Przemyslaw Fima

9:20–10:00   Olivier Dezellus
O1   IS Al-Al$_3$Nb-L PERITECTIC OR EUTECTIC? A BENCHMARK OF EXPERIMENTAL METHODS (*invited talk*)
10:00–10:20   Stephanie Lippmann
O2   METASTABLE EXTENSIONS OF PHASE EQUILIBRIA
10:20–10:40   Ondrej Zobac
O3   EXPERIMENTAL PHASE DIAGRAM OF THE Al-Ge-Mg TERNARY SYSTEM
10:40–11:10   *Coffee break*

Session 2
Chair: Stephanie Lippmann

11:10–11:30   Simona Delsante
O4   Al-Zn-TM (TM = Hf, Zr) SYSTEMS: PHASE EQUILIBRIA AND EXPERIMENTAL DETERMINATION OF THERMODYNAMIC PROPERTIES
11:30–11:50   Lisa-Yvonne Schmitt
O5   THERMODYNAMIC STUDY OF THE BINARY P-Pt SYSTEM
11:50–12:10   Wenhao Ma
O6   THERMODYNAMIC ANALYSIS AND MODELING OF NOVEL TERNARY Ni-S-BASED BULK METALLIC-FORMING SYSTEMS
12:10–12:30   Ioana Nuta
O7   THERMODYNAMICS OF THE Ag-Zr SYSTEM
12:30–14:30   *Lunch*

Session 3
Chair: Simona Delsante

14:30–14:50   Shao Wei
O8   THE PREDICTION OF Al-Li PHASE DIAGRAM BY FIRST PRINCIPLES CALCULATIONS AND STATISTICAL MECHANICS SIMULATIONS
14:50–15:10   Jan Vřeštál
O9   THERMODYNAMIC ASSESSMENT OF THE SYSTEM Nb-Sb
15:10–15:30   Pavel Brož
O10   EXPERIMENTAL STUDY AND THERMODYNAMIC MODELLING OF THE Hf-Mn SYSTEM

15:30–15:50   Hans Flandorfer
O11   ENTHALPY OF FORMATION OF SnS AND SnS_2 DEPENDING ON CRYSTAL SIZE

15:50–16:10   Andreas Leineweber
O12   SYSTEMATICS OF Sn-RICH TRANSITION-METAL ALLOYS
16:10–16:30   *Coffee break*
16:30–19:00   **Poster session**

Wednesday, 14 September 2022

Session 4
Chair: Juergen Brillo

9:00–9:40   Guy Makov
O13   PRESSURE DEPENDENCE OF BINARY PHASE DIAGRAMS: EXPERIMENTS AND THERMODYNAMIC MODELLING (*invited talk*)
9:40–10:00   Andreas Czerny
O14   HETEROGENEOUS PHASE EQUILIBRIA IN THE Mo-Si-Ti SYSTEM AT 1300°C
10:00–10:20   Hirotoyo Nakashima
O15   EXPERIMENTAL STUDY AND THERMODYNAMIC MODELING OF THE Ti–Al–Ni TERNARY SYSTEM IN THE REGION UP TO 35 AT.% Ni
10:20–10:40   Augustin Flores
O16   EXPERIMENTAL STUDY AND THERMODYNAMIC MODELING OF THE Cr–Fe–Mo–Ti SYSTEM
10:40–11:10   *Coffee break*

Session 5
Chair: Guy Makov

11:10–11:30   Juergen Brillo
O17   MOLAR HEAT CAPACITY OF LIQUID Ti, $Al_{20}Ti_{80}$ AND $Al_{50}Ti_{50}$ MEASURED IN ELECTROMAGNETIC LEVITATION
11:30–11:50   Lucas Tosin Paese
O18   ASSESSMENT ON THE Li-Ni-Mn-Co-O SYSTEM AND APPLICATIONS ON LITHIUM-ION BATTERIES LAYERED CATHODES
11:50–12:10   Magda Pęska
O19   CAST AND MECHANICALLY ALLOYED MAGNESIUM – NOBLE METALS ALLOYS AND THEIR HYDROGEN STORAGE PROPERTIES
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O20   THE PARALLEL TANGENT METHOD CORRECTED
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Session 6
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9:40–10:00 O22	Theresa Davey MIGRATION OF ALLOYING ELEMENTS AND FORMATION OF INTERMETALLIC PHASES BETWEEN CHROMIUM-BASED AND ZIRCONIUM-BASED ALLOYS (*on-line*)
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12:30–14:30	*Lunch*

Session 8
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14:30–14:50 O29	Manuel Loeffler PHASE EQUILIBRIUM INVESTIGATIONS AND THERMODYNAMIC MODELLING OF THE ZrO_2-Ta_2O_5 SYSTEM
14:50–15:10 O30	Sabina Kovaříková Oweis MODELLING OF TAU PHASES IN THE Al-Cu-Zn SYSTEM (*on-line*)
15:10–15:30 O31	Joonho Lee THERMODYNAMIC INVESTIGATION OF VANADIUM OXIDES IN CAO-SIO2-VOX SYSTEM EQUILIBRIATED WITH Pt-V ALLOYS AT 1873 K
15:30–16:10 O32	Dongwon Shin FIRST-PRINCIPLES THERMODYNAMICS OF ALUMINUM ALLOYS (*invited talk, on-line*)

SCIENTIFIC PROGRAMME

16:10–16:40   *Coffee break*

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Chair: Joonho Lee

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 O33   DESTABILIZATION OF THE ω_O PHASE OF THE Ti-Al-Nb SYSTEM BY Mo AND W ADDITIONS
17:00–17:20   Paul Lafaye
 O34   CRYSTAL CHEMISTRY AND THERMODYNAMIC MODELLING OF THE $Al_{13}(Fe,TM)_4$ SOLID SOLUTIONS (TM = Co, Cr, Mn, Ni, Pt, V)
17:20–17:40   Arkadiusz Zydek
O35   OXIDATION OF ALUMINUM-MAGNESIUM SURFACE BY REACTIVE MOLECULAR DYNAMICS STUDY
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O36   THERMODYNAMIC AND PRACTICAL ASPECTS OF CARBON CAPTURE IN MOLTEN SALTS (CCMS) TECHNOLOGY

Friday, 16 September 2022

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O42   "A JOURNEY TO THE CENTER OF A VACANCY" FREE ENERGIES OF METAL VACANCIES IN CUBIC CARBIDES
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O43   VANADIUM-BASED MISFIT LAYER COMPOUNDS: SYNTHESIS, CHARACTERISATION AND PHASE EQUILIBRIA

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Tuesday, 13 September 2022

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THE PHASE DIAGRAMS Mn-Rh AND Bi-Mn-Rh

P2   Dragan Manasijević
STUDY OF THERMAL PROPERTIES AND MICROSTRUCTURE OF THE Ag–Ge ALLOYS

P3   Ljubisa Balanović
THERMAL TRANSPORT PROPERTIES AND MICROSTRUCTURE OF THE SOLID Bi-Cu ALLOYS

P4   Ha Eun Kim
IN-SITU OBSERVATION OF PHASE TRANSITION OF SILICO-FERRITE OF CALCIUM AND ALUMINUM BY HYDROGEN REDUCTION

P5   Adam Dębski
CALORIMETRIC STUDIES OF THE Mg-Pt SYSTEM

P6   Danilo Alencar De Abreu
EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC MODELING OF THE Li_2O-Al_2O_3 SYSTEM

P7   Viera Homolova
AN UPDATED THERMODYNAMIC DESCRIPTION OF THE B-Fe-V SYSTEM WITH FOCUS ON TERNARY PHASE

P8   Marian Drienovsky
MICROSTRUCTURE EVOLUTION IN Ga-Co-Cr-Ni-Fe SERIES OF MULTIPRINCIPAL ELEMENT ALLOYS

P9   Marian Drienovsky
MICROSTRUCTURE AND THERMAL PROPERTIES OF Sn-Ag-Cu-Bi LEAD-FREE SOLDER ALLOYS

P10   Lukas Fischer
SEMI-LIQUID METAL ANODES FOR Li-ION BATTERIES: CONSTITUTION AND THERMODYNAMICS OF THE SYSTEMS Li-Zn AND Li-Sn-Zn

P11   Fabrizio Valenza
ZIRCONIA-HEA JOINTS FOR BIOMEDICAL APPLICATIONS: THE ROLE OF Ag-BASED FILLERS ON INTERFACIAL REACTIVITY

P12   Guido Kreiner
PECULIARITIES OF THE Fe-Ga SYSTEM

P13   Ivona Černičková
HIGH-TEMPERATURE PARTIAL ISOTHERMAL SECTIONS OF Al-Pd-Co PHASE DIAGRAM

P14   Libor Ďuriška
DESCRIPTION OF THERMODYNAMIC PROPERTIES OF SAC + X (X = Bi, Ga, Ni) SOLDER JOINTS

P15   Marcela E. Trybula
BEHAVIOUR OF METAL/LIQUID INTERFACES WITHIN ATOMISTIC SIMULATIONS

P16   Kamila Limanówka
EFFECT OF Er AND Zr MICRO- ALLOYING ELEMENTS ON THE STRENGTHENING OF Al-Mg ALLOYS WITH HIGH CONTENT OF Mg AFTER THERMO-MECHANICAL PROCESSING

SCIENTIFIC PROGRAMME

P17   Yuheng Liu
        SPINODAL DECOMPOSITION OF Fe-Co-Cr ALLOY AFTER ULTRA-RAPID COOLING IN POWDER BED
        FUSION ADDITIVE MANUFACTURING: A PHASE-FIELD STUDY
P18   Klaudia Walaszczyk
        ANALYSIS OF THE TEMPERATURE DISTRIBUTION ON THE SURFACE OF RECTANGULAR
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P19   Pedro P. Ferreira
        GENERALIZED QUASICHEMICAL THEORY APPLIED TO GAPLESS SYSTEMS
P20   Joonbum Park
        KINETICS OF SILICON CARBIDE DISSOLUTION IN MOLTEN IRON
P21   Rada Novakovic
        ROM BULK TO SIZE-DEPENDENT MELTING PROPERTIES OF Ag-Au NANOALLOYS
P22   Simona Delsante
        NANOTECHNOLOGY IN BIOMEDICAL APPLICATIONS: Ag/TiAlV LONG-TERM STABLE
        NANOSTRUCTURED INTERFACES FOR DENTAL IMPLANTS
P23   Alexander Westbye
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        MOLTEN SALT WITH CaO AT ELEVATED TEMPERATURE
P24   George Kaptay
        MELTING OF NANO-CRYSTALS TAKING INTO ACCOUNT SURFACE MELTING
P25   Viera Homolova
        EXPERIMENTAL STUDY OF PHASE COMPOSITION OF IRIDIUM ALLOYS
P26   Seung-Hyeok Shin
        DEVELOPMENT OF SEISMIC RESISTANT HIGH-STRENGTH LOW-CARBON DUAL-PHASE STEEL PLATE
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P27   Sang-Gyu Kim
        EFFECT OF Si CONTENT ON HYDROGEN EMBRITTLEMENT OF TEMPERED MARTENSITIC STEELS
P28   Tilen Balaško
        INFLUENCE OF CARBIDE TYPES ON THE HIGH-TEMPERATURE OXIDATION KINETICS OF HOT-WORK
        TOOL STEELS
P29   Stephanie Lippmann
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P30   Ilona Jastrzębska
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        MATERIALS FOR THE COPPER INDUSTRY
P31   Ilona Jastrzębska
        HOW FACTSAGE SOFTWARE CAN FACILITATE WORK IN REFRACTORY MATERIALS SCIENCE

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18th Discussion Meeting on Thermodynamics of Alloys

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KRAKOW

ABSTRACTS

O1

IS Al-Al$_3$Nb-L PERITECTIC OR EUTECTIC? A BENCHMARK OF EXPERIMENTAL METHODS

O. Dezellus[1], B. Gardiola[1], A. Antoni[2], A. Pisch[2], M. Barrachin[3], G. Mikaelian[4], P. Benigni[4]

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The literature agrees that the solubility of Group IV (Ti, Zr, Hf) and group V (V, Nb, Ta) elements in liquid Aluminium is very low, below 0.1 at.%. Moreover, the reported temperature of the invariant reactions involving the Al-FCC solid solution and the ε-Al$_3$M aluminides are close to the melting temperature of pure aluminium within a few kelvins. As a consequence, the nature of the invariant reaction, eutectic or peritectic is difficult to ascertain. For example, Janghorban et al.[1] reported a eutectic nature for Al-Al$_3$Zr using a specific bidifferential thermal analysis technique while Dezellus et al.[2] reported a peritectic one using the immersion-and-settling technique. Recently, Pisch et al.[3] performed calorimetric measurements of the enthalpy of dissolution of Al$_3$Nb in liquid Al and deduced a minimal value of the solubility limits that is in agreement with the values reported by Wicker et al.[4] but not with the last Calphad assessment performed by Witusiewicz et al.[5].

In the present study, several experimental techniques have been used in order to investigate the nature of the Al-Al$_3$Nb-L invariant reaction. The merits of each technique are compared allowing general recommendations for future studies.

References:

1. A. Janghorban et al., "Phase Equilibria in the Aluminium-Rich Side of the Al-Zr System", J. Therm. Anal. Calorim. 112 (2013) 301-305.

2. O. Dezellus et al., "On the Solubility of Group IV Elements (Ti, Zr, Hf) in Liquid Aluminum Below 800°C', J. Phase Equilib. Diffus. **35** (2014) 120–126.

3. A. Pisch, A. Pasturel, "On the partial enthalpy of mixing of Nb in liquid Al", Thermochimica Acta 671 (2019) 103-109,

4. A. Wicker et al., Contribution à l'étude du diagramme de phases NbAl$_3$-Al., C.R. Acad. Sci. 272C (1971) 1711–1713.

5. V.T. Witusiewicz et al., "The Al–B–Nb–Ti system: IV. Experimental study and thermodynamic re-evaluation of the binary Al–Nb and ternary Al–Nb–Ti systems", Journal of Alloys and Compounds 472 (2009) 133-161.

METASTABLE EXTENSIONS OF PHASE EQUILIBRIA

O2

S. Lippmann

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CALPHAD allows the prediction of metastable equilibria. However, the predictive power of metastable phase equilibria has limitations since the phase description itself relies on experimental data of a system in thermodynamic equilibrium. There are cases where experimentally observed phase equilibria do not agree with the predicted metastable phase equilibria. One example is the Al-Cu system in Fig.1. The metastable extensions of the fcc/liquid phase equilibria suggest a peritectic reaction that was never observed experimentally. As a workaround, the solidification community uses estimated phase diagrams for their modelling, a prominent examples is that of Gill and Kurz. It has the advantage of avoiding the peritectic reaction but reproduces the unrealistic curvature change of the solidus line in the thermodynamic description and is therefore limited in undercooling.

In the present work, the thermodynamic description of the fcc phase in the Al-Cu system has been optimized based on experimental results using electromagnetic levitation and modelling results describing the free growth of a dendrite in the diffusion-controlled regime. The revised metastable phase diagram avoids the short-comes of the previous descriptions and allows the prediction of undercoolings up to ΔT=421 K below the eutectic temperature.
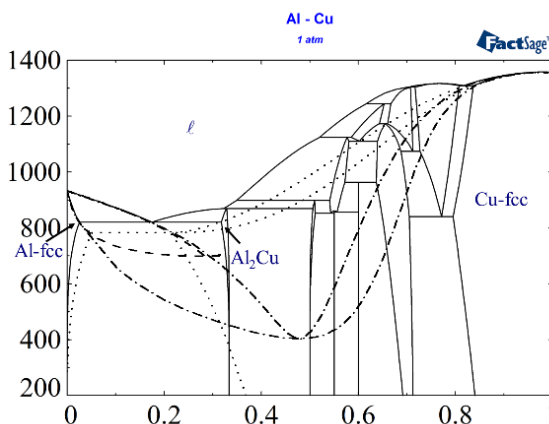

Fig. 1 Al-Cu equilibrium phase diagram (solid lines), metastable extensions of the fcc/liquid phase equilibria using SGTE 2020 database (doted lines), estimated metastable extensions (dashed lines) and optimized metastable fcc/liquid equilibria (dash-dot lines).

References:

Y. Fang, P. K. Galenko, D. Liu, K. Hack, M. Rettenmayr, S. Lippmann Phil. Trans. R. Soc. A 380 (2021) 20200327.

O3

EXPERIMENTAL PHASE DIAGRAM OF THE Al-Ge-Mg TERNARY SYSTEM

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[2] Department of Chemistry, Masaryk University, Brno, the Czech Republic.

The Al-Ge-Mg ternary phase diagram has been experimentally studied in recent decades due to its possible use in the aerospace and automotive industries. Recently, Pukas has experimentally identified a ternary intermetallic phase τ (with MgAl2Ge2 composition) [1] and a crystal structure of structure type $CaAl_2Si_2$. The theoretical assessment was performed by Islam et al. [2] before the ternary phase was found by [1]. Islam calculated two sections along the $Al-Mg_2Ge$ and $Al_3Mg_2-Mg_2Ge$ lines and compared them with the pseudo-binary sections experimentally determined by Badaeva and Kuznetsov [3]. However, the ternary phase could not be included in the theoretical sections of the phase diagram and therefore a good agreement between experiment and calculation was not achieved.

In this work, ternary Al-Ge-Mg alloys were long-term annealed at temperatures of 250, 300, 400 and 450 °C. Their microstructure, phase composition and overall composition were studied using SEM-EDX. The crystal structure of the phases was identified by XRD. Subsequently, isothermal sections of the Al-Ge-Mg experimental phase diagram at given temperatures were constructed in this study. The ternary compound τ discovered by Pukas et al. [1] was found at all annealing temperatures. It was found that the composition of the ternary phase is richer in Mg compared to the composition reported in [1]. Ternary solubility in binary intermetallic phases is negligible. The solubility of Al and Mg in Ge solid solution is significant and does not correspond to the data from the Al-Ge and Ge-Mg binary diagrams. Experimental results and data for binary subsystems were used for theoretical assessment of this system by CALPHAD method.

References:

1.   Pukas S. Pylypchak L., Matselko O., Demchenko P., Gladyshevskii R., Chem. Met. Alloys, 5/1-2, (2012), 59-65.
2. Islam F., Thykadavil A.K., Medraj M., J. Alloy. Compd, 425, (2006), 129-139.
3. Badaeva T.A., Kuznetsova R.I., Tr. Inst. Metall im. A.A. Baikova, Akad. Nauk SSSR, (3), (1958), 216-230.

Al-Zn-TM (TM = Hf, Zr) SYSTEMS: PHASE EQUILIBRIA AND EXPERIMENTAL DETERMINATION OF THERMODYNAMIC PROPERTIES

O4

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Al-based alloys have a wide range of application ranging from materials for the automotive industry going through the aerospace application to structural materials [1]. Cubic $L1_2$ (c$P4$-AuCu$_3$) trialuminides have long been of interest because of their possible use as low density, high-temperature structural materials [2] and for their possible use as precipitates for high-temperature, creep-resistant Al-based alloys [3]. It is well known that the design of new alloys requires accurate knowledge of the thermodynamic stability of all relevant phases which may be integrated within CALPHAD formalism to calculate binary and ternary phase diagrams and phase transformation driving forces. In this work we have investigated two ternary systems characterized by presence of a cubic $L1_2$ phase TM(Al,Zn)$_3$ (TM = Zr, Hf) showing a wide range of existence. Our focus was on the experimental measurement of the $\Delta_f H°$ at 300K by a calorimetric method [4] of the $L1_2$ cubic phase and about the determination of the phase equilibria. Composition and state of all investigated samples were carried out by means of Light Optical Microscopy, Scanning Electron Microscopy coupled with Energy-dispersive X-ray spectroscopy and X-ray Powder diffraction analysis.

References:

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O5

THERMODYNAMIC STUDY OF THE BINARY P-Pt SYSTEM

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Platinum phosphides are in the scope of research on platinum-based bulk metallic glasses [1] and conventional as well as glassy catalyst material [2,3]. The recently assessed binary P-Pt phase diagram is based on a study of W. Biltz and F. Weibke from 1935, which presents the experimental data of two stoichiometric phases and three types of non-variant phase transitions: an eutectic, a peritectic and a monotectic reaction [4,5]. In a previous work Differential Thermal Analysis (DTA) was performed in order to provide a general overview of the experimental performance and the non-variant phase transformation temperatures [6]. The constitutional study of the Pt-P system is experimentally challenging due to the evaporation of phosphorus during alloying, but also during the DTA measurement. The determined peritectic temperature was not in accordance to the literature. A detailed experimental update on the system is obviously needed as well as the determination of thermodynamic data for further thermodynamic optimization.

Hence, the first step of this study focuses on the optimization of the experimental condition and the detection of calorimetric data. For the annealing and the thermal analysis, the samples were sealed in fused silica crucibles in order to avoid evaporation of phosphorus, oxidation and sample-crucible reactions. These samples were measured by Differential Scanning Calorimetry (DSC) in the as-cast and the thermodynamic equilibrated state.

1. The enthalpy of each non-variant phase transformation was obtained. For several equilibrated samples the specific heat capacity could also be detected.

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THERMODYNAMIC ANALYSIS AND MODELING OF NOVEL TERNARY Ni-S-BASED BULK METALLIC-FORMING SYSTEMS

O6

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In this work, the novel Ni-Pd-S bulk metallic glass (BMG) system is studied with combined CALPHAD (CALculation of PHAse Diagram) and experimental approaches. A thermodynamic database for the Ni-Pd-S system is first developed with an association model based on the critical literature review. In addition, key experiments are performed for the examination of the phase boundaries, and for the investigation of thermophysical properties at eutectic composition and two intermetallic compositions ($Ni_{9.54}Pd_{7.46}S_{15}$ and $Ni_{3.77}Pd_{1.20}S_4$). The calculated isothermal sections and phases transition temperatures show good agreements with the experimental results.

The modelling of the undercooled liquid and the glass state take into account the heat capacity data obtained by DSC measurements of samples at various glass forming compositions. The two-state model[1] is applied for the description of the liquid-amorphous phases of pure elements. The model is then extended to its corresponding ternary system, where the modeled results are compared with experimental data and optimized accordingly. The description for the liquid-amorphous phase is used for the estimation of the driving force for nucleation at different compositions, which contributes as a vital factor for the evaluation of the glass forming ability.

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O7

THERMODYNAMICS OF THE AG-ZR SYSTEM

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Thermodynamic data for the Ag-Zr system are key elements in the calculation of strenght of materials in severe nuclear accidents.

In the Ag-Zr system, the proposed optimization by our group highlighted the need for new experimental data to give more details on the activities in the solution phases. The present study shows new data obtained by Knudsen effusion method for the sections: Ag+AgZr ; AgZr-AgZr2 ;Ar-Zr. The results are compared with the critical analysis of thermochemical data based on available published experimental data. A complete critical review and reinterpretation of data is presented in this work with a proposal of new and accurate data on Ag-Zr system.

THE PREDICTION OF Al-Li PHASE DIAGRAM BY FIRST PRINCIPLES CALCULATIONS AND STATISTICAL MECHANICS SIMULATIONS

O8

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In this work, a mean of the cluster expansion formalism in combination with semi-grand Monte Carlo was used to obtain the thermodynamic properties of Al-Li system. Firstly, the bond length-bond stiffness(L-S) relationship of different bcc and fcc configurations is obtained from transferable force constants approach by ATAT software, the accuracy of vibrational free energy and phonon density of state provide a favorable support for this method. Then, the temperature-dependent effective coefficient interaction of fcc and bcc lattice structure and ground state phases were obtained using cluster expansion formalism. The ground state phases located on the convex hull at different temperatures are Al, Al_3Li (δ'), AlLi (δ), Al_2Li_3, $AlLi_2$, Al_4Li_9 and Li, which includes all possible phases in the Al-Li alloy. Finally, the thermodynamic potentials and Gibbs free energy of the ground state phases were calculated by thermodynamic integration in Monte Carlo simulation. The inclusion of vibrational entropy was found to substantially affect the phase boundary calculation. Particularly, the combination of configurational entropy and vibrational entropy finally makes Al_3Li to be a metastable phase, which provide a new method for explaining metastable phase transition in binary system. The Al-AlLi two-phase region is observed, the composition of AlLi is correctly estimated. And the vibration disorder also makes the stability of $AlLi_2$ to be more reliable, which provides an evidence for preparing the new Al-Li alloy.

O9

THERMODYNAMIC ASSESSMENT OF THE SYSTEM Nb-Sb

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The system Nb-Sb is an important part of the Fe-Nb-Sb system, which serves as the ternary basis for excellent thermoelectric materials such as $FeNb_{1-x}T_xSb$ (T=Ti,Zr,Hf,V....). Modelling of the system Nb-Sb was performed by CALPHAD method based on the Gibbs energy data for pure elements [1]. The experimental study of the Nb-Sb system by Failamani et al. [2] verified the results of the work of Melnik et al. [3]. Our recent investigations of the Nb-rich part - covering the melting point and homogeneity region of Nb_3Sb - revealed a line compound for Nb_3Sb extending at 950°C from 75.3 at.% Nb to 74.0 at.% Nb (EMPA-WDX data). Modelling parameters based on published experiments and supported by the ab initio calculations of stability of binary structures and new experiments were determined in this work. The calculated binary phase diagram is presented in Fig.1a) and compares well with the experimentally determined one in Fig. 1b). The thermodynamic database is added.

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Fig.1.Phase diagram Nb-Sb calculated in this work, a), and in experimental work of G.Melnyk et al.,b)
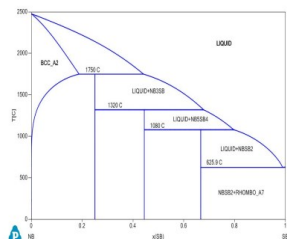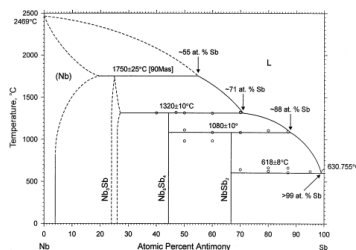
a)   b)

EXPERIMENTAL STUDY AND THERMODYNAMIC MODELLING OF THE Hf-Mn SYSTEM

O10

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A long-time interest exists for the Hf-Mn system due to the existence of the intermetallic $HfMn_2$ phase (Laves phase C14) and the HfMn phase, both candidates for hydrogen storage materials. Although structural and thermodynamic properties of the C14 phase have been investigated and exactly characterized by means of *ab initio* calculations [1], there is still a lack of reliable information on the respective phase diagram, particularly as the phase "HfMn" (sometimes described as "Hf_2Mn") is suspected to be oxygen stabilized. The existing thermodynamic assessment by Zhou et al. [2], based on the then available experimental phase and thermodynamic information and a limited set of data by the authors, creates a good basis for further studies of the binary system.

In this work, a reinvestigation of Hf-Mn phase equilibria was performed on a series of experimental alloys employing diffusion zones, thermal analysis, powder and single crystal X-ray analyses, analytical electron microscopy as well as physical property studies of the Laves phase (specific heat, electrical resistivity, magnetic susceptibility and mechanical properties). The new data were used for the thermodynamic reassessment of the Hf-Mn system. The results are discussed in view of all available information in the literature.

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O11

ENTHALPY OF FORMATION OF SnS AND SnS$_2$ DEPENDING ON CRYSTAL SIZE

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Tin sulfides, essentially SnS and SnS$_2$, are used as pigments, additives for brake linings, in photoelectric applications, as catalysts and, more recently, as anode materials for Li-ion batteries. Especially for the latter application, the grain and particle size are crucial, which in turn is significantly influenced by the manufacturing process. For the development of new batteries, the modeling and simulation of electrode reactions is of strongly increasing importance. In order to generate corresponding basic experimental data that include the energetics of the surfaces, the enthalpies of formation of SnS and SnS$_2$ from two different manufacturing methods, precipitation and hydrothermal synthesis, were investigated. Indirect drop solution calorimetry was used to determine the enthalpy of formation of the present compounds. Tin was used as the bath material. For the calculations, the limiting partial enthalpy of solution of sulfur in tin also had to be determined, since no literature data are available.

There are numerous literature data on the enthalpies of formation of the tin sulfides SnS, Sn$_2$S$_3$ and SnS$_2$. These are basically consistent yet diverge well outside the error limits. It is interesting to note that the enthalpy of formation of the three tin sulfides given for one mol of atoms is very similar, although the mutual coordination spheres of Sn and S differ. Our results for SnS and SnS$_2$ are well reproducible and within the range of literature data. The energetic differences between micro- and nanocrystalline materials are quite discernible in the trend but are barely outside the error limits.

SYSTEMATICS OF Sn-rich TRANSITION-METAL ALLOYS   **O12**

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The 3d, 4d and 5d transition-metal elements M (except for Zn/Cd/Hg) have typically high melting points in contrast to Sn with 232°C. This typically results (for high Sn contents) in a cascade of peritectic reactions which lead to the formation of intermetallic phases and to a steep decreasing the liquidus curve with increasing M content.

The present contribution will present results from the Co–Sn, Cu–Sn, Fe–Sn, Nb–Sn, Ni–Sn and Ta–Sn systems concerning formation of the Sn-rich intermetallics having the – often only approximate – formulas Cu_6Sn_5, Ni_3Sn_4/$NiSn_4$, $CoSn_3$, $NbSn_2$ and $TaSn_2$. While all systems have been investigated in view of the relevance of these systems for soldering processes and formation of superconducting compounds, it was tried to improve the knowledge by a *combination* of:

- **Phase equilibria investigations***:* The investigation of the mechanism and the kinetics of phase transformations occurring in the respective system. Including information about the kinetics of the processes leading to the equilibrium state and possible relevance for metastable or transient states.
- **Crystal structure analysis:** Measurement of lattice parameters which are a precise indicator for compositional changes.
- **First-principles calculations** (energies and structure parameters): These calculations were performed by cooperation partners or obtained from the literature.

The activities lead to a more physically reasonable description of the considered systems by the CALPHAD method, where the sublattice models of the crystalline phase are related with the insights from crystal structure analysis. The talk will focus mainly on the Cu–Sn system with respect to different forms of Cu_6Sn_5 (see e.g. Ref. [1]). The results obtained in this compositional region are discussed in view of other related systems.

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O13

PRESSURE DEPENDENCE OF BINARY PHASE DIAGRAMS: EXPERIMENTS AND THERMODYNAMIC MODELLING

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The experimental construction of phase diagrams requires accurate and well equilibrated thermo-physical measurements to obtain the equilibrium thermodynamic conditions. Hence, it took the community many decades to map the phase space of thousands of binary systems at ambient conditions. Pressure affects phase diagrams both by altering the interactions, which control the nature of the diagram, and through the emergence of new phases and phase boundaries. However, measuring thermophysical properties under pressure is challenging due to technical difficulties in pressure cells, pressure and temperature gradients which make it hard to locate phase transitions. Therefore, it is useful to combine experimental measurements and thermodynamic modelling to explore the pressure evolution of binary systems.

In the present contribution we study the pressure evolution of several binary systems through a combination of experimental techniques and thermodynamic modelling. Specifically, we studied the isomorphous Bi-Sb and the eutectic Ga-In alloy systems and were able to construct phase diagrams up to several GPa of these alloys. Our measurements include sound velocity and density at ambient pressures, x-ray diffraction in diamond anvil cell (DAC), resistivity and differential thermal analysis (DTA) in Paris-Edinburgh (PE) large volume press. These results validate our thermodynamic model of the pressure dependence of the systems; including changes in the nature of the diagram from isomorphous to eutectic, shifts of eutectic points and the evolution of interaction parameters with pressure.

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HETEROGENEOUS PHASE EQUILIBRIA IN THE Mo-Si-Ti SYSTEM AT 1300 °C

O14

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Contemporary high-temperature alloys for gas turbines operate at 90% of their melting point, necessitating the development of novel materials that withstand higher temperatures. Promising possibilities are alloys located in the system Mo-Si-Ti-B, which have been under investigation for several years and show viable properties in terms of high-temperature mechanical properties and corrosion resistance.

The group of Chang et al. [1] developed a thermodynamic database, which is widely used for CALPHAD-type analyses to guide the development of the materials system. Based on new results, some areas of the phase diagram warrant further investigation. This contribution aims to refine the thermodynamic phase modelling in the metal-rich area of the Mo-Si-Ti diagram, which is important for future applications. For this reason, several additional alloys with varying compositions were produced by vacuum arc melting from high-purity raw materials. After annealing for at least 300 h at 1300 °C and subsequent quenching, the samples were characterized via SEM, EDX and WDX to compare experimental and calculated results.

While several regions could be verified, other parts of the phase diagram need to be reevaluated. Particularly, the solubility of the (Mo,Ti) solid solution for Si is much higher than previously reported. In accordance to the new findings, the location of the technologically relevant two phase and three phase regions of the system need to be readjusted. It is likely that the difference between previously reported results and the new findings stems from quenching the samples in this study. In previous investigations, all samples were furnace-cooled, which appears to have a significant influence on the phase composition and microstructures.

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O15

EXPERIMENTAL STUDY AND THERMODYNAMIC MODELING OF THE Ti–Al–Ni TERNARY SYSTEM IN THE REGION UP TO 35 at.% Ni

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The Ti-Al-Ni ternary system is of great importance in the repair, joining, and powder processes for Ti-Al alloys. Nevertheless, there is a lack of experimental data on phase equilibria at temperatures above 1273 K, as pointed out by Schuster [1]. In this study, the TI-Al-Ni ternary system has been studied experimentally and assessed thermodynamically by the CALPHAD approach. Using six equilibrated alloys, partial isothermal sections in the composition region adjacent to the central part of the Ti-Al binary were established over the temperature range between 1673K and 1273K, by electron probe micro analyzer equipped with wavelength dispersive spectrometer. Two transition peritectic reactions of L + α-Ti = β-Ti + γ-TiAl and L + γ-TiAl = β-Ti + C14, and one transition peritectoid reactions of β-Ti + γ-TiAl = α_2-Ti$_3$Al + C14 were clarified. Based on the experimental data obtained in this work, the thermodynamic description of the Ti–Al–Ni system was newly developed.

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EXPERIMENTAL STUDY AND THERMODYNAMIC MODELING OF THE Cr–Fe–Mo–Ti SYSTEM

O16

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Cobalt constitutes a large part of the radioactive waste in the primary circuit of nuclear reactors. Replacement of cobalt-based hard coatings has been the subject of research for many years in nuclear applications. Up to now, there is no alloy capable to withstand abrasion and corrosion at 350°C and 150 bar pressure during long cycles. Complex concentrated alloys constituted by Cr-Fe-Mo-Ni-Ti have shown promising properties for these applications [1].

The Calphad method was chosen to obtain the most interesting compositions of this system. For this purpose, a critical evaluation of all constitutive subsystems was carried out. Since this system has several Frank-Kasper phases (σ, μ, χ, R, Laves), models were discussed and chosen depending on the crystal structure. Lattice stability and formation enthalpy of stable and metastable compounds were calculated by DFT. It has also been found that some systems lack reliable data or that contradictions are present in the literature. Therefore, experimental determination of phase equilibria in these systems was carried out. Samples of the Cr–Mo–Ti system were synthesized to determine the phase boundaries of the Laves phases and the extension of the Cr–Mo miscibility gap in the ternary system.

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O17

MOLAR HEAT CAPACITY OF LIQUID TI, AL20TI80 AND AL50TI50 MEASURED IN ELECTROMAGNETIC LEVITATION

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Temperature dependent isobaric molar heat capacity c_P was measured in a containerless way for liquid Ti and two AlTi binary liquid alloys. The technique of electromagnetic levitation was used in combination with laser modulation calorimetry.

In all cases, linear temperature dependencies were found: At the corresponding liquidus temperatures, c_P equals 49.75(±2.0) $J \cdot K^{-1}mol^{-1}$, 57.43(±2.9) $J \cdot K^{-1}mol^{-1}$, and 42.60(±2.2)$J \cdot K^{-1}mol^{-1}$, for Ti, Al20Ti80 and Al50Ti50, respectively. The respective temperature coefficients amount to -1.67·10^{-2}J·K^{-2}mol^{-1}, -2.73·10^{-2}J·K^{-2}mol^{-1}, and +7.83·10^{-2}J·K^{-2}mol^{-1}. For liquid Ti, there is a good agreement with existing literature data. The results are discussed in relation to the Neumann-Kopp rule

ASSESSMENT ON THE LI-NI-MN-CO-O SYSTEM AND APPLICATIONS ON LITHIUM-ION BATTERIES LAYERED CATHODES

O18

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The cathode with a layered structure most commonly used in lithium-ion batteries is the NMC (that stands for nickel, manganese and cobalt as transition metals), which belongs to the chemical system Li-Ni-Mn-Co-O. As we aim for higher capacities and greener energy technology, there is a desire to reduce the cobalt content while maintaining the battery integrity and performance. Our goal is to develop, using the CALPHAD method, a thermodynamic model of this system that will enable the search for optimal NMC compositions in terms of performance and stability.

In this study, databases of ternary Li-metal-oxides[1,2,3] were used as starting point to develop an database for the whole system based on the phase diagram data as well as the crystallographic and thermodynamic data of the relevant compounds. Preliminary results show that, for two different families of NMCs ($LiNi_xMn_xCo_{1-2x}O_2$ and $LiNi_{0.8-y}Mn_yCo_{0.2}O_2$), the model predicts with good accuracy the stabilizing character of manganese. We are also able to calculate curves of tension in function of the state of charge for a series of NMCs compositions with quite good precision. This includes surfaces of tension to respective states of charge and compositions of $Li_xNi_yCo_{1-y}O_2$ obtained with TC-Python at room temperature.

Nevertheless, input experimental data for CALPHAD modeling regarding nickel and manganese-rich compounds inside the NMC system are very scarce. To enrich the thermodynamic model, we will carry heat capacity measurements of Ni-rich compounds and ab initio calculations that will give us thermodynamic data to improve our model. Future work also comprehends further exploration of optimal Ni-rich cathode compositions and investigation on phase transitions, such as cathode degradation with formation of spinel and rock salt phases along with oxygen release.

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O19

CAST AND MECHANICALLY ALLOYED MAGNESIUM – NOBLE METALS ALLOYS AND THEIR HYDROGEN STORAGE PROPERTIES

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The issues related to the synthesis of Mg-Ag, Mg-Pd, Mg-Pt, and Mg-Pd-Ag alloys are presented in this work. The problems arising from the presence of the multiphase microstructures due to segregation during the casting are shown and discussed. Mechanical alloying in a planetary ball mill followed by annealing is proposed as the solution for this . By this method, many binary and ternary intermetallic phases were successfully synthesized. The interactions of chosen magnesium-based alloys with hydrogen are shown and discussed. The kinetics of the hydrogenation process depends on the composition of the alloy as well as it is also influenced by the shape and appearance of the powder particles that are hydrogenated. Most of the alloys were found to react with hydrogen with the formation of magnesium hydride and stable intermetallic compound as a product. Moreover, the properties of the magnesium hydride formed in such a way are almost independent of the source material composition.

THE PARALLEL TANGENT METHOD CORRECTED

O20

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The parallel tangent method widely applied to predict the composition and driving force to form a nucleus from an oversaturated solution is corrected in this paper. The parallel tangent method is shown to i). over-estimate the composition of the first nucleus, ii). neglect the concentration dependence of interfacial energies and iii). neglect the concentration dependence of probabilities to form embryos prior to nucleation (see previous ideas by Malakhov et al, [1]). New model equations are developed here for the concentration dependence of the interfacial energies and probability to form the embryos as function of nucleus composition. The most probable composition of the nucleus is found at the maximum of the driving force of nucleation corrected by the new model equations. The success of the corrected method is demonstrated on Al-Fe liquid alloy with 0.3 w% of Fe to predict the sequence of nucleation of intermetallic phases upon cooling after nucleation of the fcc phase. It is shown that although the prediction based on the parallel tangent method contradicts experimental observations, the prediction based on our corrected method agrees with them.

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O21

CALPHAD INTEGRATED DENSITY-BASED PHASE DIAGRAM AND OPENING POSSIBILITIES FOR GRAIN BOUNDARY ENGINEERING

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Engineering grain boundaries demands a quantitative description of both their segregation and specific phase behavior. Recently I have proposed a density-based model for grain boundary thermodynamics that enables CALPHAD integrated derivation of grain boundary phase diagrams [1], broadly applied now in studying various alloys [2-6]. Combining this model with experimental investigations, in this talk, new aspects of interfacial segregation and phase transformation revealed in polycrystalline alloys are discussed. The effect of elastic interaction on grain boundary phase behavior is incorporated. We consider Al alloys and novel high-entropy alloys and discuss a general strategy for grain boundary engineering.

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MIGRATION OF ALLOYING ELEMENTS AND FORMATION OF INTERMETALLIC PHASES BETWEEN CHROMIUM-BASED AND ZIRCONIUM-BASED ALLOYS

O22

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In order to improve the safety and lifetime of boiling water-type nuclear fission reactors, new accident tolerant fuels are in development where a Cr-alloy coating may be

Fig. 1: Schematic of oxidation of a Cr-alloy coating applied to Zr-alloy nuclear fuel cladding.

applied to the conventional Zr-alloy cladding on the nuclear fuel. When exposed to steam in a high-temperature accident scenario, a Cr_2O_3 scale will form on the surface, preventing catastrophic oxidation of the zirconium alloy, as shown in Figure 1. Following application of a Cr-alloy coating to the cladding, an undesirable brittle intermetallic layer of $ZrCr_2$ may form between the chromium alloy coating and the zirconium alloy cladding, damaging the integrity of the fuel system. Furthermore, diffusion of chromium, zirconium, and other alloying elements will occur in each of the metallic layers, affecting their thermodynamic and mechanical properties which may be unfavourable for the application.

The stability and structural properties of each of the layers were investigated at 0 K and finite temperature under various doping conditions using density functional theory (DFT) calculations. Spin-polarisation effects were included to capture magnetic contributions, and phonon calculations were performed to obtain the thermal-vibrational contribution to the free energy. The effects on the stability and volume of doping bcc chromium, hcp and bcc zirconium, and C15, C36, and C14 Laves phase $ZrCr_2$ with light elements, all 3d and selected 4d transition metals, and some other elements of interest was explored. The local electronic environment and chemical bonding was examined close to various dopant species in order to determine trends affecting the properties. The thermodynamics of the several layers and interfaces within the coating-cladding system were considered simultaneously to predict atomic migration and intermetallic formation within the system. Based on this data, candidate alloying elements for the Cr-alloy or Zr-alloy are proposed that may limit the formation of the $ZrCr_2$ intermetallic phases, eliminate significant volume changes that may cause microcracking, or that may improve the properties of the cladding system as a whole.

O23

DIFFUSION AND GROWTH OF β-Ni(PtPd)Al BOND COAT ON Ni-BASED SUPERALLOY

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Composition-dependent interdiffusion coefficients in multi-component systems were practically impossible until recently. The pseudo-binary (PB) and pseudo-ternary (PT) diffusion couple methods can be the choice to solve this problem. These approaches have a unique application with respect to determining the influence of alloying elements on the diffusion coefficients. Following the PB method, the impacts of Pd and Pt on the PB interdiffusion coefficients of the Ni-Al system are consistently evaluated. Pt addition is shown to accelerate interdiffusion. Pd addition was found to be less effective on the interdiffusion kinetics in Ni-Al. Similarly, the combination of these elements on diffusion in four-component β-Ni(PdPt)Al alloys are analyzed, too. The thermodynamic interactions are found to be less important, while the defect concentrations are likely to dominate the diffusion mechanism in this system. Growth rates of the interdiffusion zone between these alloys and CMSX-4 superalloys were found to follow similar trends with respect to the impact of Pd and/or Pt alloying on the calculated interdiffusion coefficients. The complex microstructure consisting of TCP precipitates in the interdiffusion zone were characterized with the help of TEM and APT.

DIFFUSION AND ATOMIC MOBILITY FOR FCC Ni-Si-Ti ALLOYS

O24

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The Ni-Si-Ti system plays an important role in high temperature structural materials. Accurate atomic mobilities of fcc Ni-Si-Ti system are essential for the microstructure simulation of Ni-based superalloys. In the present work, diffusion couples of fcc Ni-Si-Ti system have been prepared and annealed at 1273 K, 1373 K and 1473 K. By combining solid/solid diffusion couples with the electron probe microanalysis (EPMA) technique, the interdiffusivities in fcc Ni-Si-Ti were calculated via Matano-Kirkaldy method and numerical inverse method, respectively. Based on the reliable thermodynamic description and interdiffusion coefficients measured above, two sets of atomic mobilities were optimized by means of the CALTPP (CALculation of ThermoPhysical Properties) program. These atomic mobilities can reasonably describe the diffusion behaviors by comparing model-predicted diffusivities, concentration profiles and diffusion paths with the experimental ones. Besides, based on the presently obtained atomic mobilities, three-dimensional surfaces for the interdiffusivity at 1273 K, 1373 K and 1473 K were plotted. Furthermore, three-dimensional planes of the activation energy and frequency factor were evaluated using the Arrhenius equation.

O25

COMPREHENSIVE UNDERSTANDING OF DIFFUSION IN THE TERNARY CuFeNi SYSTEM: EXPERIMENTS AND THEORY

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Radiotracer diffusion of ^{59}Fe, ^{64}Cu, and ^{63}Ni was measured in selected compositions of the ternary system Cu-Fe-Ni at the temperature of 1271 K. For each composition, copper diffuses fastest while nickel is the slowest component in the system. As the Cu content in the alloys increases, all diffusivities increase, too. Such behaviour correlates well with the successive lowering of the melting temperature of the corresponding alloys with increasing Cu content. The radiotracer measurements are combined with the novel augmented tracer-interdiffusion couple approach which uses the same set of alloy materials for the diffusion couples. The tracer-interdiffusion couple method facilitates the estimation of the composition-dependent tracer diffusivities using a single diffusion couple. The results confirm the high level of reliability and reproducibility of this approach for producing highly accurate diffusion data for generating mobility databases. Together with CALPHAD-like theoretical analysis these results present a complete data set for the quantitative verification of any theoretical description of diffusion in ternary alloys. Finally, the impact of vacancy generation on the tracer and chemical diffusion in the concentration gradient is analysed.

PHASE-FIELD SIMULATION OF ANTIPHASE DOMAIN GROWTH FOR $D0_3$ ORDERED Fe_3Al ALLOY

O26

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[Introduction] The mechanical or magnetic properties of the ordered phases are closely related to the antiphase domain (APD) structures, such as the APD size and the characteristics of antiphase domain boundaries (APBs). For example, it has been reported that pseudoelasticity is caused in Fe_3Al by the interaction between APBs and dislocations [1]. Phase-field (PF) simulation has been proved to be an effective way of studying the formation and time-evolution of APD for ordered phases. Koizumi et al. [2] studied the ordering mobility in nearly stoichiometric Fe_3Al at constant temperatures by the PF method. The objective of this study is to develop PF simulations applicable to temperature variations for the APD growth in $D0_3$ ordered Fe_3Al alloy, aiming at the optimization of aging conditions for ordering in the future.

[Methods] PF simulations of ordering in Fe-28at.%Al alloy were performed for the cases of constant cooling rate and isothermal aging. The dimension of the simulation domain area was a cube with a size of 30 nm. Thermodynamic equilibrium at 873 K was assumed as the initial state for all simulations. The evolution of $D0_3$ APD during cooling to 673 K at rates of 0.1~1000 K/s and that during aging at constant temperatures of 673 K, 723 K, and 773 K for 1 h after cooling at 100 K/s were examined and compared with experimental results.

[Results] The simulation results for the case of constant cooling rate showed that the growth of the $D0_3$ APD takes place before the detectable long-range order (LRO) appears. Moreover, slower cooling rates resulted in larger APD sizes. On the other hand, although the ultimate LRO obtained by isothermal aging at a lower temperature is higher than that at a higher temperature, $D0_3$-LRO exhibited a significant increase earlier in aging at higher temperatures. Besides, the growth of $D0_3$ APD also begins earlier when aging at higher temperatures, which is due to the larger ordering mobility at the higher temperature. In conclusion, isothermal aging at higher temperatures after cooling at a higher rate is considered suitable for the fast growth of $D0_3$ APD in the Fe_3Al.

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O27

DEVELOPMENT OF ALUMINA-BASED THERMODYNAMIC DATABASE FOR AL MELT FILTRATION

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The alumina-based ceramic foam filters are proposed for Al melt filtration process in order to remove oxide inclusions. In the context, the influence of different filter surface chemistries (Al_2O_3, spinel $MgAl_2O_4$, mullite $3Al_2O_3 \cdot 2SiO_2$, SiO_2, and TiO_2 coatings) on the properties of Al_2O_3-based foam filters was discussed and their filtration efficiencies were evaluated [1,2]. For instance, rutile coatings deposited on corundum were supposed to filtrate actively and reactively spinel $MgAl_2O_4$ and Al_2O_3 inclusions present in Al alloy melt. The experiments performed using Al alloy containing Mg and Si indicated formation of $MgTiO_3$ phase and absence of Al_3Ti phase [3]. However, $Ti_5(Si,Al)_3$, $Ti(Al,Si)_3$ and ternary phases could form. Therefore, thermodynamic database of the complex Al–Ti–Mg–Si–O system is essential to develop a tool for optimizing the conditions during interfacial reactions between the filter and the Al-based alloy melt. The oxide part of Al_2O_3–MgO–TiO_2–SiO_2 is of interest. To model the system using the CALPHAD approach, the compound energy formalism was used to describe the solid solutions and a two-sublattice partially ionic model was used for the liquid phase. The model parameters were optimized by using PARROT-Module of the Thermo-Calc Software. The thermodynamic descriptions of the Al_2O_3–MgO–TiO_2, Al_2O_3–TiO_2–SiO_2, and Al_2O_3–MgO–SiO_2 systems are accepted from the previous works or from the literature. For the MgO–TiO_2–SiO_2 system, all three pseudo binary sub-systems are available. In this work, the MgO-TiO_2-SiO_2 system was investigated experimentally to verify the literature data and assessed thermodynamically.

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THERMODYNAMIC MODELLING OF THE Al_2O_3-CaO-FeO_x SYSTEM

O28

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Al_2O_3, CaO, Fe_2O_3, and FeO are the main components in industrial solid wastes such as red mud and coal gangue, and the Al_2O_3-CaO-FeO_x system is also an important slag system in the metallurgical industry. Knowledge of phase equilibria on the Al_2O_3-CaO-FeO_x system is very important for the resource utilization of industrial solid waste and the metallurgical processes.

In the present work, the thermodynamic assessment of the Al_2O_3-CaO-FeO_x system was carried out based on the available data by means of the CALPHAD(calculation of phase diagrams) method. The subsystems Al_2O_3-CaO, CaO-FeO_x, and Al_2O_3-FeO_x were partially assessed by the previous Refs [1-3]. All the solid solution phases were described using the compound energy formalism. Besides, the liquid phase was described by the ionic two-sublattice model, $(Al^{+3}, Fe^{+2}, Ca^{+2})_P(AlO_{1.5}, FeO_{1.5}, O^{-2}, VA)_Q$. And the intermetallic compounds, including $2CaO \cdot 3Fe_2O_3 \cdot Al_2O_3$ and $CaO \cdot (Al_2O_3, Fe_2O_3)_3$ were treated as stoichiometric phases. A good agreement between the calculated results and experimental data is obtained. The presently obtained thermodynamic parameters for the Al_2O_3-CaO-FeO_x system are of great interest for the development of the Al_2O_3-CaO-SiO_2-MgO-Fe_2O_3-FeO-Na_2O multicomponent system.

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18th Discussion Meeting on Thermodynamics of Alloys TOFA 2022, 12-16 September 2022, Krakow

O29

PHASE EQUILIBRIUM INVESTIGATIONS AND THERMODYNAMIC MODELLING OF THE ZrO_2-Ta_2O_5 SYSTEM.

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To increase efficiency of stationary and aircraft engines by increasing temperature new materials for thermal barrier coating (TBC) applications are searched. The oxidic materials in ZrO_2-HfO_2-$YO_{1,5}$-$TaO_{2,5}$ system (Pitek und Levi 2007; Lepple et al. 2019) present interest due to their stability at high temperature and other properties suitable for TBC. A fundamental understanding of thermodynamics of this system is necessary for future practical applications. In the ZrO_2-$TaO_{2,5}$ system as one of sub-system of the multi-component system experimental data on phase equilibria were limited. Therefore, it was necessary to investigate phase equilibria in this system and measure thermodynamic properties in order to obtain thermodynamic description of the ZrO_2-$TaO_{2,5}$ system. The derived thermodynamic description will be used to develop thermodynamic database of high order system ZrO_2-HfO_2-$YO_{1,5}$-$TaO_{2,5}$. The samples in the ZrO_2-$TaO_{2,5}$ system with compositions in the range from 14.28 mol.% up to 95 mol.% of Ta_2O_5 were prepared using coprecipitation reaction of $TaCl_5$ and Zr-acetate in presence of NH_3OH. In a next step precipitates were dried, calcinated, pressed and sintered. Sintering as heat treatment were performed at different temperatures from 1400 °C up to 1700 °C. The samples were characterized by SEM/EDX, XRD, DTA and DSC. Especially the intermediate phase $Ta_2Zr_6O_{17}$ was of particular interest for further measurements of heat capacity. Lattice parameters were determined using Rietveld Analysis. The already reported crystal structures of phases in the system were mostly confirmed. However, for the Ta_2O_5 phase we found a more uncommon monoclinic distorted variant of the orthorhombic high temperature phase at 1600 °C and 1700 °C. The more common tetragonal low temperature phase was present at 1400 °C. Microstructural studies were performed using SEM/EDX. The temperatures of phase transitions and melting relations were investigated in single-phase and two-phase regions. Heat capacities and enthalpies of transformations were determined using DSC. These thermodynamic and phase equilibrium data are used for modelling the Gibbs energies of the phases in the particular system. Based on the obtained information the preliminary thermodynamic database using CALPHAD modelling has been derived.

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MODELLING OF TAU PHASES
IN THE Al-Cu-Zn SYSTEM

O30

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We have performed a combined theoretical and experimental study of two allotropes of the tau phase in the Al-Cu-Zn system. Quantum-mechanical calculations and CALPHAD modelling were employed in combination with experimental data (SEM, DTA, XRD) [1]. Thermodynamic, structural and elastic properties have been investigated in the case of both rhombohedral and cubic allotropes of the tau phase. The supercell approach was used to model the composition $Al_{13}Cu_{10}Zn_2$ with 1/6 of the total number of atomic positions vacant. The quantum-mechanical calculations performed using the VASP code provided the energies of formation of the end-members of the rhombohedral tau phase, which form the solid base for the phase-diagram modelling. The rhombohedral allotrope reveals higher stability with respect to the fcc Al and Cu and hcp Zn than the cubic one. The volume per atom of the cubic phase is bigger than that of the rhombohedral phase by 0.54 %. Elastic constants of both allotropes indicate their significant elastic stiffness. Furthermore, the stability and vibrational entropy of the cubic and rhombohedral modification of this phase were studied using phonon-spectra calculations within the quasi-harmonic approximation resulting in the temperature dependence of the total Gibbs free energy, equilibrium volume, heat capacity, bulk modulus, etc.

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O31

THERMODYNAMIC INVESTIGATION OF VANADIUM OXIDES IN CAO-SIO$_2$-VO$_X$ SYSTEM EQUILIBRIATED WITH PT-V ALLOYS AT 1873 K

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Owing to the complexity of the multi valence states of vanadium oxides in slag systems and experimental difficulties, thermodynamic properties of vanadium oxides have not been established yet. In the present study, the mixed-valence states and activities of the vanadium oxides in CaO-SiO$_2$-VO$_x$ slag were investigated experimentally at 1873 K and oxygen partial pressures of 3.2×10^{-9} and 3.1×10^{-7} atm. After the CaO-SiO$_2$-VO$_x$ slag had equilibrated with a platinum strip, the mixed-valence states of the vanadium oxides in the slag were estimated by performing X-ray photoelectron spectroscopy, and the activities of the vanadium oxides in the slag were calculated using the activity of vanadium in the platinum strip at equilibrium using thermodynamic equations. At an oxygen partial pressure of 3.2×10^{-9} atm, V^{3+} was the dominant ion and V^{4+} was the second most abundant ion. With increasing VO$_x$ content or basicity (CaO/SiO$_2$ ratio), the fraction of V^{3+} decreased, whereas that of V^{4+} increased. The activity of VO$_{1.5}$ was greater than those of the other vanadium oxides. On the other hand, when the oxygen partial pressure increased to 3.1×10^{-7} atm, V^{4+} became the dominant ion. As the slag basicity increased, the fraction of V^{4+} increased further, whereas that of V^{3+} decreased to less than that of V^{5+}. The activity of VO$_{1.5}$ was greater than those of the other vanadium oxides, limiting the effect of the slag basicity. Consequently, the valence state of vanadium oxide was affected by the slag basicity at a low oxygen partial pressure by acting as a network modifier. In contrast, at a higher oxygen partial pressure, the activity of vanadium oxide increased further but was not affected by the slag basicity because of its contribution to the network structure formation. The present findings can be applied to optimize the slag composition in steel refining or vanadium pentoxide production processes to increase the yield rate of vanadium.

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FIRST-PRINCIPLES THERMODYNAMICS OF ALUMINUM ALLOYS

O32

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Due to the relatively shorter research history, the amount of data for aluminum alloys are far smaller than their counterpart, i.e., iron and steel. While it is a preferred and ideal method of data acquisition for alloys, relying on sole experimental measurements of the thermodynamic properties of alloys is discouraged in modern materials science research. Also, some critical properties at lower length-scales can be more efficiently derived via theoretical investigation. In this presentation, I will introduce how modern high-performance computing combined with advanced characterization techniques can rapidly populate reliable data that can be readily used to design aluminum alloys for automotive applications. Examples include the energetics of solute segregation at the interface between the aluminum matrix and key precipitates and solute-solute-vacancy clustering in the aluminum matrix. The research was sponsored by the U.S. Department of Energy, Vehicle Technologies Office, Propulsion Materials Program.

O33

DESTABILIZATION OF THE ω_o PHASE OF THE Ti-Al-Nb SYSTEM BY Mo AND W ADDITIONS

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Light-weight LPT (low-pressure turbine) blades employed in modern jet engines for service at high temperatures are made of alloys that are mainly based on the Ti-Al-Nb system. In the composition range relevant to the urgently needed development of improved alloys, the ternary equilibrium phase "Ti_4NbAl_3" (usually designated as the ω_o phase) occurs, which is detrimental to the materials' properties due to its embrittling effect and should be avoided. It is known that there is no corresponding equilibrium phase in the related systems Ti-Al-Mo and Ti-Al-W, and it can therefore be expected that the addition of Mo or W to Ti-Al-Nb alloys will reduce the amount and/or stability of the ω_o phase. However, there are no systematic studies on this issue. Here we present some results on the effect of additions of 1-5 at.% Mo or W on the stability of the ω_o phase.

The research was carried out within the scope of the CleanSky 2 EU-project ADVANCE, which aims at improving an existing CALPHAD database of related materials systems to speed up the development of next-generation TiAl-based alloys.

CRYSTAL CHEMISTRY AND THERMODYNAMIC MODELLING OF THE Al$_{13}$(Fe,TM)$_4$ SOLID SOLUTIONS (TM = Co, Cr, Mn, Ni, Pt, V)

O34

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The Fe content in Al alloys is usually tightly tracked in order to control the precipitation of brittle Al-Fe intermetallic compounds such as the Al$_{13}$Fe$_4$ intermetallic phase (*C2/m*). This intermetallic can have detrimental effects on the mechanical behaviour of aluminium alloys by forming crack initiation sites [1-2]. For other applications, the presence of Fe in aluminium alloys is promoted to improve their corrosion resistance and to increase their hardness [3]. Moreover, several alloying elements such as Co, Cr, Mn, Ni, V [4] can be added to the material to refine the coarse structure of the Al$_{13}$Fe$_4$ precipitates and to strengthen the material. In this context, it is of prime importance to better predict the thermodynamic stability of this phase as a function of both the temperature and the chemical composition. In this study, the crystal chemistry of the Al$_{13}$(Fe,TM)$_4$ (TM = Co, Cr, Mn, Ni, Pt, V) solid solutions has been investigated by combining new formation enthalpy measurements by differential scanning calorimetry (DSC), new density functional theory (DFT) calculations and thermodynamic modelling. The formation enthalpies of seven alloys of the Al$_{13}$(Fe,Co)$_4$ solid solution were measured by DSC at 920 K, allowing the determination of the mixing enthalpy of the solution. The formation enthalpy of six alloys belonging to the Al$_{13}$(Fe,Mn)$_4$ and Al$_{13}$(Fe,V)$_4$ solid solutions were also measured by DSC at 920 K. These measurements are presented here for the first time. In addition, the mixing enthalpy of the Al$_{13}$(Fe,TM)$_4$ solid solutions (TM = Co, Cr, Mn, Ni, Pt, V) was determined by DFT at 0 K. These new calculated and measured data were used to perform the thermodynamic modelling of the solid solutions and to calculate the TM occupancy on the Fe sites of the Al$_{13}$(Fe,TM)$_4$ solid solution structure at different temperatures. The crystal chemistry characterisation of the Al$_{13}$(Fe,TM)$_4$ solid solutions performed in this framework allowed us to quantify their chemical ordering as a function of temperature but also to design an optimal sub-lattice (SL) model for all these solid solutions.

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O35

OXIDATION OF ALUMINUM-MAGNESIUM SURFACE BY REACTIVE MOLECULAR DYNAMICS STUDY

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Al-Mg alloys are an important and gaining popularity branch of materials due to the combination of such features as: good strength, low density and good resistance to atmospheric corrosion. These alloys are widely used in industry including automotive, aerospace, defense and marine industries. Al alloys with a content of less than 5%at. Mg, which have very good corrosion resistance in ambient conditions, are of particular interest. However, resistance to this type of corrosion decreases significantly with increasing temperature. Therefore, there is a need to investigate the mechanisms of Al-Mg alloy corrosion in dry environment by considering different factors such as oxygen gas concentration and temperature. Reactive molecular dynamics is an ideal method to simulate corrosion mechanisms because it can account for the formation and breakdown of atomic bonds in formed oxides. This technique will help understand the early stages of surface corrosion.

In this contribution, we discuss atomistic simulations results confronted with available experiment performed for thermal oxidation of aluminum-magnesium alloy [1]. Molecular dynamics simulations based on the reactive force field, ReaxFF, was performed at selected temperatures according to phase diagram [2]. Structure and chemistry of oxide thin films grown on Al-Mg surface during corrosion in dry environment was investigated computing chemical composition, bond length and respective structural properties of thin film. To inspect in detail structure of both thin film and Al-Mg substrate, Voronoi analysis were performed. Kinetics of thin film grown upon dry corrosion was also inspected computing thickness and effective diffusion coefficient to assess the corrosion rate. The obtained results allowed to conclude that the thickness of the formed oxide layer increases with the oxidation temperature increase. The obtained results allow to get atomic level insight on into the mechanism of oxide formation on Al-Mg alloy's surface and describe kinetics together with structure and respective properties of thin films.

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THERMODYNAMIC AND PRACTICAL ASPECTS OF CARBON CAPTURE IN MOLTEN SALTS (CCMS) TECHNOLOGY

O36

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The capture and storage of CO_2 emitted from exploitation of fossil fuels has been identified as an issue, which should be resolved immediately. It is related to the observed, dangerous climate changes on Earth, which are caused by greenhouse gases, mainly CO_2. One of the effective method of capturing CO_2 from diluted gases is the carbonate looping method. The process is based on the carbonation reaction of MO with CO_2 and decarbonation of the formed MCO_3. Particularly, the Calcium Looping technology (CaL) persists as an economically and environmentally attractive high-temperature CO_2 capture process. The most disadvantage of solid state Ca-looping is the decreasing sorbent reactivity after many absorption-desorption cycles. Avoiding sorbent degradation is possible through a process known as Carbon Capture in Molten Salts (CCMS). In this process the active substance (CaO) is present as dissolved or partially dissolved, in a liquid consisting of molten inorganic halide salts. The most promising salt mixture is eutectic $CaCl_2$-CaF_2, as the solvent for the dissolution/dispersion of CaO and $CaCO_3$. Results achieved to date indicate extremely efficient absorption and high absorption rate in molten salts based on such a systems. From the practical point of view, the process requires the knowledge of the molten salts viscosity. It is expected that the CaO and the $CaCl_2$-CaF_2 form a slurry due to supersaturation of CaO. This will lead to increase in viscosity, which could be a challenge in a scaled-up system where a possible approach is to transfer/pump the melts between the absorber and the desorber chambers. In order to take these possible limitations into account, an experimental evaluation of the viscosity of the $CaCl_2$-CaF_2-CaO-$CaCO_3$ system was performed. Tests were performed at 750 ÷ 950°C for $CaCl_2$-CaF_2 eutectic system and various content of CaO and $CaCO_3$ (5÷35 wt.%). The obtained results indicate a slight change in viscosity as a function of both the temperature and the tested CaO and $CaCO_3$ concentrations. The system was difficult to study due to the presence of CaO and $CaCO_3$ in suspended form and observed sedimentation. The highest viscosity obtained for a system with 35 wt.% of CaO was not more than 60 cP. This viscosity should not hinder the transport of the molten salt between the absorption and desorption chambers during the continuously process.

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O37

CHARACTERIZATION AND MODELING OF THE CHEMICAL COMPOSITION OF GROWING GRAIN BOUNDARY CEMENTITE IN HYPEREUTECTOID STEELS

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Prediction of grain boundary cementite growth kinetics in hypereutectoid steels is a question of major industrial importance. Mechanical properties of the alloy deteriorate with greater cementite thickness. New modelling approaches were recently suggested for significantly improved simulation of grain boundary cementite thickness over time in steel with up to three elements [1]. In the present work, we present chemical analysis of grain boundary cementite in multi-component hypereutectoid steels at different stages of isothermal cementite growth, using Electron Probe Micro Analysis (EPMA) data. These experimental results are then compared to simulations of cementite precipitation using a modification of SFFK model within MatCalc [2], which can account for heterogeneous site nucleation energy [1]. The model parametrization for complex steels is validated by comparison of the predicted cementite thickness with experimental results. Parameters include an assessment of the multi-component thermodynamic equilibrium and the diffusion mobilities database (Matcalc tdb and ddb databases), the choice of the cementite precipitate character (para- or ortho-equilibrium), and the consideration of diffusion to and within grain boundary cementite (this is particularly relevant at long reaction times). The discussion aims on the solution to the question: how can we model correctly the influence of alloying elements on grain boundary cementite growth in complex systems?

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EXPERIMENTAL INVESTIGATION OF SOLID-LIQUID EQUILIBRIA IN THE Fe-B BINARY SYSTEM FOR LOW BORON CONTENTS

O38

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High-strength steels grades contain small amount of boron, less than 40 ppm by mass, in order to suppress liquid metal embrittlement. During solidification in continuous casting, the formation of slab defects could be originated from a metatectic type transformation of ferrite δ into austenite γ, leading to a retrograde melting during cooling [1]. However, existing thermodynamic databases, which could support the optimization of the elaboration conditions, do not cover composition and temperature ranges considered for the targeted application. For example, for the Fe-B binary system, according to literature data, the maximum solubility of B is 97 ppm or 970 ppm in the ferritic phase and 25 ppm or 390 ppm in the austenitic phase with a difference of more than 30°C in the value of the metatectic reaction temperature, without any experimental arguments being available to explain these differences [2].

This study focuses on the establishment of new solid-liquid experimental data in the Fe-B binary system, for boron content ranges below 1000 ppm. Two types of experiments are carried out: (i) measurements by differential thermal analysis and (ii) thermal treatments involving the liquid phase by means of electromagnetic phase separation technique. Phase stability domains, solidification paths and microstructure morphology are characterized by SEM and X-ray diffraction. Due to the low boron solubility values expected in the phases, especially in the ferritic or austenitic solid solutions, accurate characterisation methods are required to obtain their compositions. This is achieved by using GD-OES, ICP, EPMA-WDS measurements supplemented by SIMS analyses. A comparison of the different methods of characterisation used is given and our findings are discussed.

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O39

THE THERMODYNAMIC MODEL OF THE TERNARY FE-MN-SI AND ITS IMPACT ON THE QUATERNARY FE-MN-SI-C FOR PREDICTION OF PHASE EQUILIBRIA IN NEW STEEL GRADES OF THIRD GENERATION

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In order to develop new steel grades of third generation with high alloying contents of elements like Mn and Si, a good knowledge of phase equilibria in Fe-rich side chemical systems with these elements is required, and it goes without saying that consistency of available data on phase equilibria from different sources need verification before building a thermodynamic model. In this context, the most recent assessments of the ternary system Fe-Mn-Si have been evaluated on the basis of the available experimental data from literature. Then, the impact of the ternary model on phase equilibria in the quaternary system Fe-Mn-Si-C has been studied. Such system is very crucial for predicting the correct solidification sequences around the peritectic domain in steels of third generation.

THERMODYNAMIC MODELLING OF STEEL RECYCLING

O40

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Due to the increasing demand of steel production, the reduction of primary ressources and the challenge on the environmental footprint, recycling scrap materials for the steel production is necessary. However, use of recycled materials implies to introduce solute elements and thus to increase the amount of alloying elements in the material. While, there is a real potential of using scrap materials, the presence and concentration of these tramp elements must be considered in the process, since it affects process- and product-relevant issues such as the formation of precipitates, shift of phase transformation temperatures, or segregation at grain boundaries.

In order to consider the role of tramp elements in scrap alloy materials, we use thermodynamic modeling of Fe-base multi-component systems with the impurities of Cu, Sn, As, Bi, and Zn and we analyse the effect of respective tramp elements on the equilibrium phase stabilities and thermodynamic properties. We show a number of examples of the use of Calphad methodology for the assessment of the effects of residual elements. Among these, we discuss the limits for the formation and development of uncontrolled phases due to impurities, the influence on phase transformations, as well as expected segregation during steel casting.

In the framework of applied Calphad to practical metallurgy, we also propose solutions of how to tackle the effect of residual elements by adjusting the chemical composition of the given alloy, i.e. by modulating the amount of an alloy element already present in the steel. Finally, also challenges of the Calphad methodology for interpretations of the influence of tramp elements for alloy materials are discussed.

O41

ACCESSING VACANCY SEGREGATION AT HETEROGENEOUS INTERFACES IN METAL/METAL AND METAL/CERAMIC NANO-MULTILAYERS

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Vacancies play an important role in the structure and properties of heterogeneous metal/metal and metal/ceramic interfaces. By exploring vacancy formation energy maps at incoherent interfaces in non-reactive Cu/W and Cu/AlN nano-multilayers using first-principles calculations, we access the role of interface structure and chemistry on vacancy segregation behavior, predicting the resulting mass transport in such materials at finite temperatures. Our predictions explain well experimental observations and can be used to guide further experiments to access the effect of stress and temperature on thermal stability as well as heat and mass transport properties in nanocomposite materials for heterogeneous integration in nano- and microelectronics applications.

"A JOURNEY TO THE CENTER OF A VACANCY" FREE ENERGIES OF METAL VACANCIES IN CUBIC CARBIDES

O42

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Transition metal (TM) carbides with the cubic Halite structure, such as TiC and ZrC, combine ceramic-like properties with metal-like properties, which is a desirable combination for many existing and emerging applications of these compounds [1]. TiC and ZrC have great hardness at room temperature, but soften very rapidly with increasing temperature to become as soft as the respective metals already at about 1000°C. The softening effect can be remedied (or at least delayed) in a mixed carbide system (Ti,Zr)C, due to a spinodal decomposition into an ultrafine mixture of TiC- and ZrC-enriched regions. The decomposition is controlled by the rate of metal atom diffusion, and therefore the atomic mechanism(s) and other details of metal (Me) selfdiffusion in cubic MeC compounds are of interest. This information is essential for modeling the structure and property evolution in hard materials during manufacturing and service. We employ ab initio calculations, using a plane-wave method [2] with projector augmented wave type pseudopotentials [3,4] and a gradient-corrected density functional [5], to systematically compute the energies and structures of point defects and their arrangements in MeC systems, as well as to simulate the processes of defect migration through the Halite lattice. Different mediators of Me diffusion have been considered previously, including clusters of vacancies [6,7] and interstitial atoms [8,9]. Based on the recent finding of a new (symmetry-broken) configuration of a Ti mono- vacancy in TiC that is almost twice lower in energy than the symmetric configuration. We explore the configurational space of a Me monovacancy to locate several energy minima. Among them, a planar symmetry-broken configuration with the optimal number, length, and angles of C-C bonds is found to be the global energy minimum. The formation and thermodynamic behaviour of this and other symmetry-broken configurations at elevated temperatures are essential for describing Me self-diffusion in MeC by the mono-vacancy mechanism.

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O43

VANADIUM-BASED MISFIT LAYER COMPOUNDS: SYNTHESIS, CHARACTERISATION AND PHASE EQUILIBRIA

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Starting with the discovery of the useful properties of graphene, low-dimensional materials have gained substantial interest in literature. Transition metal dichalcogenides (TMDs) like Se_2V are among the promising candidates for inorganic 2D materials to be possibly used in next-generation electronics, anode materials in lithium-ion batteries, water splitting by hydrogen evolution reaction and other potential applications. Ternary systems M−Se−V, where M can be bismuth, lead, tin or a rare earth element, might additionally host the so-called misfit layer compounds (MLCs), which are another type of 2D materials. Their crystal structure is comprising of a layered composite. The general formula of MLCs $[(MX)_{1+\delta}]_m(TX_2)_n$ reflects the fact that two interpenetrating, yet structurally different, subsystems are stacked. The TX_2 subsystem is based on the triple layer of TMDs and these layers are interspaced by a distorted sodium chloride type layer MX. Usually, the two subsystems coincide in one crystallographic direction, but are incommensurately modulated in the second. Furthermore, different stacking sequences may be observed which are described by the parameters m and n in the general formula $[(MX)_{1+\delta}]_m(TX_2)_n$.

Synthesis of such MLCs is demanding and almost nothing is known about the phase equilibria in the respective ternary systems. Information on Se_2V-based MLCs is scarce, but thin film studies indicate that they may exist as thermodynamically stable phases. In the current study we investigated the possibility of MLC bulk-synthesis in the three ternary systems (Pb,Sb,Sn)−Se−V. These efforts were combined with a systematic study of phase equilibria in the respective ternary systems. Selected phase diagram data are presented together with insights into synthesis strategies for MLCs and the characterization of compounds by means of electron microscopy and XRD methods.

CAN WE IMPROVE OUR CURRENT VIEW OF THE IRON-CARBON PHASE DIAGRAM?

O44

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To most of materials scientists nowadays, it would appear very unlikely that the Fe-C phase diagram should be improved. There are however some points to be clarified, which could prove useful in designing radically new steels. Nowadays in fact it is well accepted that the development of new alloys, including of course steels, may be carried out by a combination of software and experiments. In the sense that Calphad has been introduced by Larry Kaufman, there could be ways to attribute thermodynamic properties to phases which are nowadays still impossible or difficult to synthesize in pure form. The case of iron carbides is typical, especially for some higher carbon iron carbides. It is in fact not easy to link different and sometimes controversial informations which have been obtained, to name a few, from the Catalysis scientific community and the ab-initio community to information related to tempering of (high carbon) steels, mechanochemical synthesis and some specific phenomena like white etching layers in steels. Some commonly accepted thermodynamic databases from different authors are reviewed and compared along with a new and simple methodological approach proposed here which suggests to add to GHSER data a very simple enthalpy term, which scales with stored enthalpy – in the thermodynamic database itself.

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THERMODYNAMICS OF ALLOYS

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P1

THE PHASE DIAGRAMS MN-RH AND BI-MN-RH

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The increasing demand for rare earth elements (REEs), particularly for the production of efficient permanent magnets, may cause problems for both, cost and availability, of these elements. Therefore, an intensive search for REE-free ferromagnetic materials has taken place since several decades. The compound α-BiMn is among the promising candidates. It crystallizes in the hexagonal NiAs (B8) type structure and is stable up to 355 ± 2°C, where it decomposes in a peritectic reaction into a Bi-rich liquid and the high-temperature non-ferromagnetic β-BiMn modification. However, due to the low peritectic melting and the slow diffusion of Bi, it is extremely difficult to produce phase pure α-BiMn. One of the strategies to overcome this problem is to search for stabilized solid solutions of third elements in α-BiMn or closely related magnetic compounds in ternary Bi−Mn based systems.

In course of a systematic investigation of corresponding ternary systems we studied Bi−Mn−Rh and also re-assessed the binary Mn−Rh system. The binary manganese-rhodium phase diagram was re-investigated experimentally from 5 to 90 at.% Rh with focus on determining the transition temperature between the ordered γ'-Mn_3Rh ($L1_2$) and the γ-Mn (A1) solid solution. The transition temperature between the $L1_0$ and B2 (β-MnRh) phases and various phase boundaries were studied applying XRD, DTA and SEM/EDX.

Phase equilibria of the ternary bismuth-manganese-rhodium system were experimentally investigated, focusing on the possible existence of new ferromagnetic phases. Isothermal sections at 330°C and 600°C were studied and the corresponding phase diagram was established based on these results.

STUDY OF THERMAL PROPERTIES AND MICROSTRUCTURE OF THE Ag–Ge ALLOYS

P2

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Microstructure, phase transitions and thermal properties including thermal diffusivity and thermal conductivity of four Ag–Ge alloys with 20, 40, 60 and 80 at.% of Ge were experimentally investigated in this study. Observation and analysis of the alloy microstructures and morphologies of (Ge) phase in the hypereutectic alloys were carried out using optical microscopy and scanning electron microscopy with energy dispersive X-ray spectrometry (SEM-EDS). Phase transitions of the alloys were studied using differential scanning calorimetry (DSC). Experimentally determined temperature of the eutectic reaction was 650.9 °C. The xenon-flash method was used for thermal diffusivity measurements in the temperature range from 25 to 400 °C. Based on the measured values of thermal diffusivity, thermal conductivity of the solid Ag–Ge alloys was determined. It was found that both thermal diffusivity and thermal conductivity show a minimum at 20 at.% Ge which is close to the eutectic composition. The obtained results were compared with the results of thermodynamic calculation and literature data and a close agreement was observed.

P3

THERMAL TRANSPORT PROPERTIES AND MICROSTRUCTURE OF THE SOLID Bi-Cu ALLOYS

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Thermal transport properties of solid Bi-Cu alloys have been studied in a wide composition range and the temperature range from 25 up to 250 °C. Thermal diffusivity was measured using the flash method. It was found that the thermal diffusivity continuously decreases with increasing bismuth content and temperature. The density of the Bi-Cu alloys at 25 °C was measured using the indirect Archimedean method. The density of alloys decreases slightly with increasing copper content. Thermal conductivity was determined based on measured diffusivity and density of alloys, as well as based on calculated specific heat capacity. Analogous to the thermal diffusivity, the thermal conductivity of the studied Bi-Cu alloys decreases with increasing bismuth content and temperature. The microstructure and melting behavior of the Bi-Cu alloys were analyzed using scanning electron microscopy (SEM) with energy dispersive X-ray spectrometry (EDS) and differential scanning calorimetry (DSC). The measured eutectic temperature was 269.9 °C. The measured phase transition temperatures and related heat effects were compared with the results of thermodynamic calculations according to the CALPHAD method.

IN-SITU OBSERVATION OF PHASE TRANSITION OF SILICO-FERRITE OF CALCIUM AND ALUMINUM BY HYDROGEN REDUCTION

P4

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Production of zero-carbon steel is highly anticipated as a sustainable solution for net-zero. Hydrogen reduction of the iron-ore sinter in the blast furnace operation is considered a promising candidate. Here, delayed molten phase formation would be problematic. In the iron ore sinter, silico-ferrite of calcium and aluminum (SFCA) is a major bonding phase, in which Fe^{2+} prefers to place at octahedral sites, while Fe^{3+} at tetrahedral sites. During the reduction in the ironmaking process, however, the phase stability and crystalline structure are modified, yielding drastic changes in the primary molten slag formation. In this study, in-situ observation of phase transformation was carried out using a confocal laser scanning microscope(CLSM). The phase transformation before and after reduction was examined using differential scanning calorimetry(DSC), separately. An SFCA sample was placed in a platinum crucible and heated under an Ar-5%H_2 gas atmosphere while investigating with CSLM. The sample was melted at 1181℃, which was similar to the result of DSC. The liquid phase region gradually expanded, but at 1330℃, the dendrite phase suddenly appeared, and the liquid phase transformed into a solid phase. When the temperature increases to 1500℃, a liquid phase is formed again overall. The present result suggests an understanding of the molten slag formation route in hydrogen-enriched blast furnace operation. (This work was supported by the Industrial Strategic Technology Development Program (20212010100040, Development of hybrid ironmaking processes for lower CO2 emissions), funded by the Ministry of Trade, Industry & Energy in the Republic of Korea.)

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P5

CALORIMETRIC STUDIES OF THE MG-PT SYSTEM

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The knowledge of thermodynamic properties is important when we design new engineering materials. Unfortunately, despite many decades of scientific work as well as improved research instruments, some of the binary phase equilibrium systems are still unknown or are only theoretically predicted or calculated. The cause of this situation often arises from the difficulties in preparing the alloys for measurements, which are caused, for example, by significant differences in the melting points of the components, their reactivity with the structural materials of the research apparatus, significant differences in densities or high vapor pressure causing intensive evaporation and sometimes even sublimation of low melting point components. For the above-mentioned reasons, alloys from the Mg-Pt system are difficult to produce, and the availability of thermodynamic data of the above system is very limited. Therefore, this work presents the calorimetric results of the mixing enthalpy of liquid Mg-Pt alloys as well as, calorimetrically determined for the first time, the standard enthalpy of formation of alloys and intermetallic phases of the Mg-Pt system. The obtained values of the integral mixing enthalpies of Mg-Pt liquid alloys were negative under the tested conditions and in the examined concentration range. In the case of the enthalpy of formation of alloys from the Mg-Pt system, from the measured heat effects, the values of the standard enthalpies of formation of alloys and intermetallic phases were determined and compared with the existing ab initio data as well as with the data calculated with the use of the Miedema model [1, 2].

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EXPERIMENTAL INVESTIGATION AND THERMODYNAMIC MODELING OF THE Li_2O-Al_2O_3 SYSTEM

P6

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The importance to recycle and recover valuable transition metals (such Co, Ni) and Li increased in the recent years. Several metallurgical methods have been investigated to obtain transition metals from their respective oxides after reduction slag separation and crystallization processes. In this process Li_2O reacts with slag forming $LiAlO_2$ or spinel solid solution. In this context, the development of thermodynamic database for the Li_2O-MnO_x-SiO_2-Al_2O_3 is an important step to create a tool to optimize conditions, at which maximal separation of Li_2O can be obtained. Thus, investigations of pseudo-ternary and pseudo-binary systems among these oxides, like the Li_2O-Al_2O_3 system, is necessary to provide some data and contribute to improve the processing conditions. The experimental investigations for selected group of heat-treated and quenched samples were carried out via microstructural characterization using Scanning Electron Microscope (SEM), Energy Dispersive Spectroscopy (EDX), X-Ray Diffractometry (XRD), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC). Considering the literature data for this system and the necessity to develop a consistent thermodynamic database using the Compounds Energy and Formalism (CEF) for solid phases as well as for the two-sublattice partially model ionic liquid, a preliminary thermodynamic modeling of the Li_2O-Al_2O_3 system is proposed in this work based on CALPHAD approach. The inverse spinel phase $(Al^{+3},Li^{+1})_1^T$:$(Al^{+3},Li^{+1},Va)_2^O$:O_4 was modeled using two cationic sublattices and its extension in Al_2O_3 composition region assuming presence of the vacancies in octahedral sites. Spinel is reversed and practically the ion Al^{+3} occupy the tetrahedral sites completely. The compound $LiAlO_2\_ht$ melts congruently. Two eutectic reactions (Ionic liq. $\rightarrow$ Li_5AlO_4 +$LiAlO_2\_ht$ and Ionic liq. $\rightarrow$ $LiAlO_2\_ht$ + Spinel), three peritectic reactions (Ionic liq. + Li_2O $\rightarrow$ Li_5AlO_4, Ionic liq. + $LiAl_{11}O_{17}$ $\rightarrow$ Spinel and Ionic liq. + Corundum$\rightarrow$ $LiAl_{11}O_{17}$), two eutectoid reactions ($LiAl_{11}O_{17}$ $\rightarrow$ Spinel + Corundum and Spinel $\rightarrow$ $LiAl_5O_8$ + Corundum) and one peritectoid reaction (Spinel + $LiAlO_2\_ht$ $\rightarrow$ $LiAl_5O_8$), as well as the polymorphic transformation ($LiAlO_2\_ht$ $\rightarrow$ $LiAlO_2\_rt$) are reproduced in the present work. The calculated phase diagram satisfactorily agrees with the experimental results.

P7

AN UPDATED THERMODYNAMIC DESCRIPTION OF THE B-FE-V SYSTEM WITH FOCUS ON TERNARY PHASE

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The boron-iron-vanadium system was experimentally studied and assessed by Homolova et al. [1]. In the mentioned work, a ternary phase was experimentally observed in the system for the first time. The ternary phase with about 40 at% of boron was described as a stoichiometric phase with three-sublattice model with formula $(V)0.32(Fe)0.28(B)0.4$. However, detailed information on this phase was missing. Later, new experimental data on the ternary phase in the system was published by Rogl et al. [2]. A crystal structure of the phase and some physical properties were determined.

In the present work, differential thermal analysis of equilibrated B-Fe-V alloy containing the ternary phase was performed. The obtained results and knowledge about ternary phase were used to improve the description of the boron-iron-vanadium ternary system.

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MICROSTRUCTURE EVOLUTION IN Ga-Co-Cr-Ni-Fe SERIES OF MULTIPRINCIPAL ELEMENT ALLOYS

P8

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Multiprincipal element alloys (MPEAs), formely also known as high entropy alloys (HEAs), are nowadays probably the most studied metalic systems [1]. MPEAs usually have very distinguishing characteristics in comparison with conventional alloys. These characteristics are given mainly by their composition and structure.

This study is based on our previous results [2] where we observed an ultrafine-structured constituent consisting of β-GaCo and β-GaCu phases. The constituent, designated as β-mixture, behaves as a single phase and its structure resembles that of superalloys. Now we mixed new GaCoCrNiFe series of alloys, where their composition of (GaNi) is as follows: 0.4, 0.7, 1.0, 1.3 and 1.6 at.%. The alloys were prepared by melting pure elements in a vacuum arc smelter under an argon atmosphere. All five alloys in as-cast state were processed for follow-up experiments, such as X-ray diffraction measurements (XRD), scanning electron microscopy observations of the microstructure with microchemical analysis (SEM-EDX), and differential thermal analysis coupled with thermogravimetric analysis (DTA-TGA).

Only two crystal structures – body-centered cubic (BCC) and face-centered cubic (FCC) were found in the all five alloys. With a growing amount of (GaNi), the fraction of BCC phase increased. The finest microstructure was observed at the composition of (GaNi) = 1.0. With an increasing content of the (GaNi), the melting temperature decreased. The alloys had a slight decrease in mass at temperatures around 1400 °C. The higher the content of Ga in the alloy was, the higher the decrease in mass was detected. Therefore, this seems to occure due to Ga element evaporation.

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P9

MICROSTRUCTURE AND THERMAL PROPERTIES OF Sn-Ag-Cu-Bi LEAD-FREE SOLDER ALLOYS

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Lead-free solders are crucial low-melting alloys for the electroctronic industry to join electronic components. The most popular alloys are those composed of Sn, Ag, and Cu (SAC) [1]. However, because of the increasing cost of Ag, manufactures and their customers prefer soldering alloys with low Ag content. An additional alloying element, such as Bi, can partially replace the expensive Ag element and improve some useful properties of the SAC alloy [2]. Using Thermo-Calc software with COST531 Lead-free solder database, we desing composition of the new low-Ag SAC alloy with various Bi additions (0, 1, 2 and 4 wt.%). This new composition is compared with the popular SAC-near eutectic alloy with the same Bi additions.

The alloys were manufactured from pure elements by melting in a vacuum induction furnace under an Ar atmosphere. After that, they were processed for initial experiments, such as X-ray diffraction analysis (XRD), scanning electron microscopy observations of the microstructure with microchemical analysis (SEM-EDX), and differential scanning calorimetry (DSC).

The composition of all aloys consist of β-Sn solid solution, Ag_3Sn, and Cu_6Sn_5. The separate Bi phase was only found in the alloys with the highest content of this element. DSC analysis shows that with increasing content of Bi in the alloys the liquidus temperature drops more than the solidus temperature, i.e. the pasty range increases. However, the enthalpy of fusion continuously decreased with growing amout of Bi in the alloy.

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SEMI-LIQUID METAL ANODES FOR LI-ION BATTERIES: CONSTITUTION AND THERMODYNAMICS OF THE SYSTEMS Li-Zn AND Li-Sn-Zn

P10

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Due to the ever-increasing energy demand and the need of constant availability of portable as well as stationary power sources there is a necessity of continuous improvement of energy storage devices. Among batteries one promising cell type is the Li-ion battery that shows several advantages, e.g. high energy densities, low self-discharge rates and high operation voltages. However, high power performance characteristics can only be satisfied based on new electrode and electrolyte materials. Conventional carbon-based anodes like graphite are abundant, cheap and persistent but suffer on poor specific capacities (372 mAhg^{-1}). Alternatives among others are intermetallic formation anodes, e.g. based on Sn. Tin is an excellent electron conductor and shows a high theoretical capacity of 994 mAhg^{-1} during lithiation (up to $Li_{4.4}Sn$). A major disadvantage, however, is crack formation on repeated charge and discharge cycles caused by large volume changes during lithiation leading to rather fast degradation of the electrode material and thus low cyclability.

Self-healing of cracks based on liquid and semi-liquid electrode materials is one solution to overcome this problem. To make use of this effect at room temperature, the melting point of the anode material must be lowered by addition of further low-melting elements, such as Bi, Ga, In and Zn. Phase diagram investigations based on XRD, SEM and thermal analysis are performed in order to understand the related electrode alloys and their lithiation. This re-assessment of intermetallic systems also includes thermochemical measurements, e.g. calorimetry. All results can be introduced into the optimization of thermodynamic Gibbs Energy models (CALPHAD). Our investigations in terms of phase equilibria started with the system Li-Zn, the only before mentioned binary with Li which is not yet fully clarified and were continued with the ternary system Li-Sn-Zn. Isothermal sections and isoplethes in Li-Sn-Zn were established and compared with a calculated phase diagram [1]. Partial and integral molar enthalpies of mixing of liquid Li-Zn [2,3] and Li-Sn-Zn alloys were investigated by drop calorimetry and fitted with a Redlich-Kister Muggianu model. In addition, the application of ternary alloys as anodes are considered. In this context the phase equilibria of the system Bi-Sn-Zn were investigated.

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POSTER ABSTRACTS

P11

ZIRCONIA-HEA JOINTS FOR BIOMEDICAL APPLICATIONS: THE ROLE OF AG-BASED FILLERS ON INTERFACIAL REACTIVITY

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Recently, Ti-based refractory High Entropy Alloys (HEA), such as TiZrTaHfNb have been proposed to replace Ti6Al4V for biomedical applications due to the harmfulness of long term release of Al and V ions. With the aim of testing the possibility to produce ceramic-to-metal seals for these systems to be adopted in implantable medical devices, in this poster we present ZrO_2-Ag-HEA joints. To this end, the system reactivity, wettability of ZrO_2 by different Ag-based alloys at 1000°C and their interfacial layers were studied. Interpretation and discussion of systems reactivity were supported by thermodynamic calculations, according to the CALPHAD approach and the ad-hoc Ag-Ti-Zr-O thermodynamic database, implemented in this work. A good wettability was reached at 1000°C adding Ti to Ag: Ag-4Ti and Ag-8Ti reached contact angles of 81-85°. Ag-4Ti-2Zr showed the best wettability (77°) and the most complex interfacial microstructure. A continuous hcp-(Ti,O) layer promoted the wettability of Ag-4Ti and Ag-8Ti. In both cases, AgTi was the only intermetallic compound found in the bulk. Ag-4Ti-2Zr formed a thicker interfacial layer of hcp-(Ti,Zr,O)+bcc-(Ti,Zr) + a less compact $Ag(Ti,Zr)_2$ layer. Here, a low amount of Ag(Ti,Zr) and $Ag(Ti,Zr)_2$ was found in the Ag matrix.

Following the results from wettability tests, joints between ZrO_2 and a $Ti_{1.5}ZrHf_{0.5}Ta_{0.5}Nb_{0.5}$ HEA were produced at 1000 °C through a pure Ag brazing filler being the active elements, Ti and Zr, provided by diffusion from the HEA. The microstructural characterization showed defects and intermetallic-free interfaces with a first layer in contact with zirconia, mainly composed of Ag, Ti and Zr (HV ~ 600) followed by a plastic Ag-based area (HV ~ 250) extending until the HEA bulk. Further mechanical and electrochemical evaluations of the system are under way to demonstrate the possibility of using HEA-Ag-ZrO_2 joints for biomedical applications.

PECULIARITIES OF THE Fe–Ga SYSTEM

P12

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The system Fe–Ga is attracting interest as low-Ga content alloys show promising magnetostrictive properties, making them possible substitutes for rare-earth containing materials, e.g., for magnetic actuators. Like its homologue Al, Ga stabilises the (bcc-base) α-Fe solid solution as compared to γ-Fe–Ga, which has, like α-Fe–Al, some B2/D0$_3$ ordering tendency. The extended α-Fe–Ga solid solution is, however, over a large compositional range, only metastable with respect to other phases, while α-Fe–Al (or its B2-ordered variant) appears to be stable up to about 50 at.% Al. It is the transformations in the Fe–Ga system, in particular the processes leading to the fcc-base L1$_2$ superstructure which are related to the magnetostrictive properties of Fe–Ga alloys in the corresponding compositional range.

At higher Ga contents (e.g. 38 at.%), the bcc-base solid solution α-Fe–Ga also appears to be metastable towards formation of an (itself metastable) intermetallic phase with ideal formula Fe$_{13}$Ga$_9$ [1]. Its monoclinic crystal structure has already been mentioned in passing previously [2] and can be regarded as an ordered and vacancy-containing variant of the ω phase, which is also confirmed by typical orientation relationship of Fe$_{13}$Ga$_9$ with the bcc matrix [1]. Hence, the bcc-base Fe–Ga phases exhibit signs of the two different modes of instability of bcc structures, i.e. the $\frac{1}{2}(C_{11}-C_{12})$ elastic instability (Bain and Burgers paths) and the L point dynamic instability (path towards ω). The current presentation puts own experimental insight into stable and metastable phase stabilities Fe–Ga system into literature context, including in particular comparison with systems like Fe–Al and Fe–Ge showing similarities towards Fe–Ga but also decisive differences. Main aim is an improvement of the overall understanding of the A2/B2/D03 type related transition-metal–main-group element phases concerning thermodynamic stabilities and vacancy formation.

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POSTER ABSTRACTS

P13

HIGH-TEMPERATURE PARTIAL ISOTHERMAL SECTIONS OF Al-Pd-Co PHASE DIAGRAM

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This work deals with the experimental study of the Al-Pd-Co system in the vicinity of peritectic formation of the ε_n quasicrystal approximant. Twelve Al-Pd-Co alloys with various chemical compositions annealed at 1035 °C were invetigated using scanning electron microscopy including energy dispersive X-ray spectroscopy and X-ray diffraction. Altogether ten phases, namely ε_n, F, Z-Al$_3$Co, β, V, δ, U, Al$_5$Co$_2$, m-Al$_{13}$Co$_4$ and liquid were present in the investigated alloys at 1035 °C. Based on the experimental results the partial isothermal section of the Al-Pd-Co phase diagram at 1035 °C was proposed [1] and compared to the earlier published partial isothermal sections at 1000 °C [2], 1020 °C [3] and 1050 °C [2]. It was found that the same ternary phases are present at isothermal sections at 1000, 1020 and 1035 °C. However, their homogeneity ranges were slightly different. The comparison of the isothermal sections at 1035 °C and 1050 °C showed that the ternary phases U, δ, and ε_n occur at 1035 °C only. Phases F and V are present at both the temperatures, while the ternary W phase occurs at 1050 °C only.

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DESCRIPTION OF THERMODYNAMIC PROPERTIES OF SAC + X (X = Bi, Ga, Ni) SOLDER JOINTS

P14

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Although a lot of work was done at investigation of SAC solders in previous years, some problems are still not solved [1]. The influence of composition and thermal treatment on growth of intermetallic compounds at substrate-solder interface becomes important in understanding the resulting microstructure and properties of solder joints [2-3]. At present phase-field modelling seems to be a very useful technique how to describe the microstructure evolution in materials at different conditions [4], if the thermodynamic and kinetic parameters of investigated systems are known. This work deals with description of thermodynamic properties of SAC + X (X = Bi, Ga, Ni) / Cu substrate solder joints using Thermo-Calc software and available data, e.g. from [5]. These results can be useful in further thermodynamic modelling of microstructure evolution during solidification and annealing in this system.

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P15

BEHAVIOUR OF METAL/LIQUID INTERFACES WITHIN ATOMISTIC SIMULATIONS

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Phenomena occurring on metal surfaces represent a vast field of basic scientific research and play a key role in the degradation of many technological materials. Atomic-level understanding of processes occurring at metal/liquid interface containing acid and alkaline substances provides the unique knowledge enabling to correctly manipulate parameters for operating processes towards inhibition of material degradation.

Reactive molecular dynamics simulations were performed to study mechanisms of film growth upon exposure of metal/oxide surface to corrosive media, including water-containing solutions enriched in H_3O^+ or OH^- ions at 363K. The particular focus was on finding the relationships between chemical, topological, and kinetic factors. A systematic study of ions concentration on the behaviour of metal/oxide surface was performed to describe structural, morphological and topological differences associated with mechanism of film growth in aqueous solutions of varied pH.

The difference is found in the mechanism of film growth on metal exposed to strongly corrosive media of different pH influences structure, surface topography, and interatomic bond topology of the films. Chemical composition of the developed films was also studied. Higher content of OH group anchored to metal/oxide surface is found in alkaline solutions which increases the surface roughness and solvent accessible surface area (SASA). Topological aspects of the grown films and metaloxide interface were described performing Voronoi analysis supplemented with *n*-ring analysis. A dominance of lattice distortions of Al substrate over crystal defects was observed and topologically complex amorphous nature of the films form rather than crystalline or liquid.

EFFECT OF ER AND ZR MICRO- ALLOYING ELEMENTS ON THE STRENGTHENING OF Al-Mg ALLOYS WIHT HIGH CONTENT OF MG AFTER THERMO-MECHANICAL PROCESSING

P16

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Al-Mg alloys are attractive due to their extremely low density and the strengthening the solid solution with magnesium. The strength of Al-Mg alloys increases with increasing concentration of Mg [1]. Moreover, they can work hardening. The recovery and recrystallization processes encountered during heat treatment decrease mechanical properties [2]. One of the ways to eliminate the decrease in mechanical properties is to introduce micro-alloying elements. The addition of Er in Al-Mg alloys increases their mechanical properties, and Al_3Er dispersoids can improve their thermal stability [3]. The addition of Zr forms Al_3Zr dispersoids which block the grain growth during subsequent deformations processes [4]. Simultaneous adding of Er and Zr to Al-Mg alloys could improve their mechanical properties and thermal stability due to densely and evenly distributed $Al_3(Er,Zr)$ dispersoids to be formed [5]. The subject of the work is the analysis of the microstructure and Brinell hardness of the Al- 7 %wt. Mg alloy and the Al- 7 %wt. Mg with Zr, Er and Er together with Zr. The influence of the micro-alloying elements on the durability of their mechanical properties after thermo-mechanical processing was analysed. Er and Zr added to the Al- 7 %wt. Mg alloy significantly reduce decrease in mechanical properties after thermo-mechanical processing. The average grain size of analysed alloys before and after thermo-mechanical processing was determined using the Zeiss Axio Observer 7 Mat light microscope. The scanning and transmission electron microscopes (SEM Inspect F50, TEM Tecnai G2) were used to characterize their microstructure and phase composition. Mechanisms of improving the durability of the alloy mechanical properties were also investigated.

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SPINODAL DECOMPOSITION OF FE-CO-CR ALLOY AFTER ULTRA-RAPID COOLING IN POWDER BED FUSION ADDITIVE MANUFACTURING: A PHASE-FIELD STUDY

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[Introduction] Fe-Co-Cr permanent magnetic alloys are attractive because of the combination of good ductility and tunable magnetic properties. The mechanical and magnetic properties of these alloys are strongly affected by the microstructures formed by the spinodal decomposition. To optimize the coercivity and remanence of the alloys, precise multiple-step aging is indispensable. Recently, the additive manufacturing of the Fe-Co-Cr alloy using powder bed fusion (PBF) has been reported. Although the segregation of brittle phases can be suppressed commonly in many alloys fabricated by PBF, solidification cellular structures and inter-cellular boundary segregation were observed occasionally [1]. Moreover, the supersaturated vacancies can be introduced by the ultra-high cooling conditions of PBF process. These characteristics of PBF may affect the spinodal decomposition reaction [2]. This study aimed to investigate the influences of vacancies on spinodal decomposition by the phase-field simulation.

[Methods] Phase-Field models taking into account the concentration of vacancies were used to simulate the spinodal decomposition for Fe-12Co-25Cr mass% alloy. The diffusivity of vacancies was assumed to decay with time. Besides, the influence of the dimension of the simulation model (the 2D or 3D) was also examined. The fractions, size, and number densities of the separated phases of the simulation result were compared with the experimental data.

[Results] Although the microstructures were qualitatively similar to the experimental ones, some discrepancies were found. The discrepancy was reduced by using 3D model. The discrepancy in the initial kinetics can be partly attributed to the supersaturated vacancies. However, it was suggested that the inaccuracy of the thermodynamic parameters is also responsible. Therefore, the thermodynamic parameters were modified. The optimization of aging conditions for the PBF process by phase-field simulation will also be discussed.

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ANALYSIS OF THE TEMPERATURE DISTRIBUTION ON THE SURFACE OF RECTANGULAR CONTINUOUS INGOTS

P18

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The technology of continuous casting of steel (CCS) is the leading industry of steel production in the world. On the quality of the steel obtained is influenced by all factors at every stage of its production, which is why the appropriate selection of materials and CCS parameters is so important. This allows to obtain semi-finished products of high quality, free from internal and surface defects. The article presents the results of tests on the temperature distribution on the surface of continuous rectangular ingots. The LANDSCAN LSP-HD 10 laser temperature scanner was used for the analysis. The device allowed for the analysis of temperature distribution and determination of the influence of temperature on the formation of defects.

Keywords: continuous casting of steel, temperature distribution, laser temperature scanner, slab

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GENERALIZED QUASICHEMICAL THEORY APPLIED TO GAPLESS SYSTEMS

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Within generalized quasichemical approximation (GQCA), an arbitrary pseudobinary alloy $A_{1-x}B_x$ is described by an ensemble of M individual clusters statistically and energetically independent of the surrounding atomic configurations with n sites that may be occupied by atoms A or B. With that, one can estimate any alloy property through an average of P_j values, obtained from quantum mechanical ab initio calculations, weighted by the probabilities x_j that minimize the overall mixing Helmholtz free energy per cluster at a given temperature and composition. This simple, but robust statistical thermodynamic model was widely used in the past for studying semiconductor systems, especially phase decomposition effects and the evolution of the energy gap between conduction and valence bands in function of the alloy composition. However, in the present work, we have applied the GQCA model to metallic systems of scientific and technological interest to easily assess the thermodynamic stability and electronic correlations on the same footing. We have focused on transition metal dichalcogenides' class (TMDs), with a particular interest in describing the intercalation effects of foreign species in between adjacent chalcogen planes that are weakly held by van der Waals interactions. Our results show that a realistic intercalated TMD alloy grown from equilibrium processes tends to crystalize homogenously. This information is crucial for manipulating alloy properties sensitive to the local environment, such as topological properties. Additionally, we show how this simple method can successfully describe more complex phenomenologies, like superconductivity, by evaluating critical parameters such as the density of states at the Fermi level and electron-phonon coupling.

KINETICS OF SILICON CARBIDE DISSOLUTION IN MOLTEN IRON

P20

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For a stable steelmaking process, it is important to properly control the Silicon concentration of molten iron in the ironmaking process. Among molten iron, Silicon has a higher affinity for oxygen than Phosporous, thus tends to be oxidized first. Accordingly, it is necessary to appropriately control the Silicon concentration in the molten iron. Meanwhile, in the sampling experiment of the existing blast furnace, it was confirmed that SiC was observed in the carbonaceous materials layer below the blast furnace.[1-2] In particular, it has been reported that SiC on the coke surface is the most notable Si-containing raw material in the raceway area of the blast furnace.[3] Therefore, it is necessary to pay attention to SiC as the cause of Si affecting the molten iron in the blast furnace, as well as to investigate Si dissolution from SiC in terms of kinetics through lab experiments. In this study, the dissolution rate of SiC in molten Fe-C alloys was investigated using sampling technique in the temperature range of 1673~1773 K, while the initial carbon concentration was varied from 2 to 3 wt%. The dissolution of SiC occurred by the carbon-saturation concentration. The dissolution rate constant increased from 8.17×10^{-3} to 18.41×10^{-3} cm/s by increasing temperature from 1673 to 1773 K, yielding the activation energy of 199.7 kJ/mol. As the initial carbon concentration increased from 2.31 to 3.07 wt%, the rate constant decreased from 8.17×10^{-3} to 2.90×10^{-3} cm/s. Sulfur concentration did not affect the SiC dissolution rates in molten Iron, so it was considered that the sulfur adsorption at the metal/SiC interface was not so significant. Based on the present experimental results, an empirical equation was suggested for the estimation of the rate constant $\ln k = 9.50565 - 1.3678 \times ([wt\%C] - 2)24019.8/T$.

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FROM BULK TO SIZE-DEPENDENT MELTING PROPERTIES OF Ag-Au NANOALLOYS

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The thermodynamic, surface and transport properties together with two macroscopic functions related to the structure of Ag-Au melts were calculated using thermodynamic models and the Quasi-Chemical Approximation (QCA) for the regular solutions, developed in the framework of statistical mechanics combined with Quasi Lattice Theory (QLT). 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 and it differs only slightly from a classic thermodynamic model based on the Butler equation, widely used to calculate the surface tension isotherm of Ag-Au melts.. A few Ag-rich Ag-Au alloys have been measured by the pinned drop method and the results were compared to the literature data as well as to the model predicted values. Ag@Au nanoalloys (10 at% Au) have been synthesized by co-reduction of aqueous solution of $AgNO_3$ and $HAuCl_4$ as precursors and ascorbic acid as reducing agent and in presence of NH_3. In order to verify composition, shape, dimension and thermal behaviour of the nanostructured samples, the following experimental techniques have been employed: X-Ray Powder Diffraction (XRPD), Field Emission Gun Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (FEGSEM) and Differential Scanning Calorimetry (DSC). The dimensions of Ag@Au nanoparticles were analysed in terms of the Ag-Au nanosized phase diagram.

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NANOTECHNOLOGY IN BIOMEDICAL APPLICATIONS: Ag/TiAlV LONG-TERM STABLE NANOSTRUCTURED INTERFACES FOR DENTAL IMPLANTS

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Titanium (Ti) based implants are commonly used in dental surgery for restoring teeth. One of the challenges in implantology is to achieve and maintain the osseointegration as well as the epithelial junction of the gingival with implants. However, oral cavity incessantly encounters a plethora of microorganisms which may affect the successful implant osseointegration [1]. Antimicrobial nanoparticles (NPs) are promising because of several advantages such as ultra-small sizes, large surface-area-to-mass ratio and special physical and chemical properties.

This paper aims to present a comprehensive investigation on the development and application of antibacterial Silver nanoparticles (AgNPs) in dentistry including restorative dentistry, endodontics, implantology, dental prostheses, orthodontics mainly based on Ti-implants. Indeed, AgNPs are able to physically interact with the cell surface of various bacteria (i.e. Gram-negative) by damaging their cell membranes [2]. On the other hand, AgNPs can easily enter the body and accumulate in organs leading to symptoms of poisoning due to the extremely small particle size [3].

For the mentioned reasons, our study focuses on designing successfully long-term stable Ag/TiAlV nanostructured interfaces by controlling interaction phenomena and adhesion. Specifically, by studying reactivity at the solid and liquid states the interaction phenomena occurring as functions of size, temperature and time at the Ag/Ti and Ag/TiAlV interfaces have been deeply examined and the results obtained are here presented and discussed both from theoretical and experimental points of view.

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CORROSION IN SELECTED CERAMICS AND NICKEL ALLOYS EXPOSED TO A EUTECTIC CaCl$_2$-CaF$_2$ MOLTEN SALT WITH CaO AT ELEVATED TEMPERATURE

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The applications of molten salts include concentrated solar power (CSP), thermal energy storage (TES), nuclear energy and industrial chemical processes. The molten salt application of relevance for the presented work is "*Carbon Capture in Molten Salts*" (CCMS), a post-combustion carbon capture concept aimed at the chemical industry, primarily flue gases from metallurgical processes. CCMS is based on a cyclic absorption/desorption temperature swing (700 - 950°C, 0.1 MPa) utilizing a eutectic calcium chloride/fluoride molten salt (86.2/13.8 wt% CaCl$_2$/CaF$_2$) with 5 – 30 wt% added calcium oxide (CaO($s,diss$)) for carbon capture through carbonate (CaCO$_3$($diss$)) formation.

CCMS is currently at TRL3/TRL4. One key issue hindering further upscaling is that of corrosion, and by extension the identification and characterization of appropriate reactor construction materials. The molten chloride/fluoride salt is highly corrosive at high temperature, and the introduction of flue gas constituents (nitrogen, carbon dioxide, steam, oxygen and varying degrees of other impurities from combustion) places further constraints on material properties. Hydrolysis from the addition of steam and formation of hydrochloric acid (HCl) poses a particularly difficult challenge, though hydrolysis can be partially suppressed by the addition of CaO. To date, the best performing material has been pure nickel. However, upon prolonged exposure to the molten salt under cyclic operation, significant grain growth excludes pure nickel as a suitable construction material.

Corrosion testing has been performed for > 20 metals and ceramics, including nickel-based "*superalloys*" (hastelloy, inconel, haynes, monel etc.) and various ceramic materials (alumina, boron nitride, silicon carbide, silicon oxide, aluminum nitride etc.). Initial material screening has been performed through "crash testing" of materials at 700°C and 900°C, whereby materials were exposed to atmospheric gas phase compositions. The best performing materials have been subjected to more detailed studies under controlled atmospheres. Samples are characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDX) and by measuring weight change. The most corrosion resistant material tested to date is Haynes 230 alloy (Ni/Cr/W).

MELTING OF NANO-CRYSTALS TAKING INTO ACCOUNT SURFACE MELTING

P24

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The surface melting of macro-crystals and melting of nano-crystal for Al, Cu and Ag pure component are modeled in comparison with literature data. The relevant temperatures of surface premelting and melting are calculated. The corresponding temperature dependent equilibrium thickness of liquid melted layer is obtained as well, which tends to infinity when temperature is at the bulk melting point. Further, the size-dependent melting behavior for Al, Cu and Ag is investigated and the critical size is determined by a home-made code. The melting point depression with particle size is also demonstrated in present work. As illustrated in size-dependent phase diagram, the temperatures of both solidus and liquidus decrease and they merge together with the radius descending.

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EXPERIMENTAL STUDY OF PHASE COMPOSITION OF IRIDIUM ALLOYS

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Iridium is an element which, due to its thermodynamic properties, is very interesting for use in the aerospace industry and due to its high corrosion resistance even at very high temperatures, it may potentially be suitable for use as part of gas turbine materials.

The subjects of the present study were Ir-Ho, Ir-Mn binary and Ir-Cr-In ternary alloys. X-ray diffraction and scanning electron microscopy equipped with EDX analyzer were used for determination of phase equilibria and composition of the coexisting phases in the iridium alloys after long-term annealing (350–1500 h) and without annealing. Also differential thermal analysis of equilibrated alloys was performed.

The results of the experimental study will be base for developed thermodynamic assessments of the binary and ternary systems.

DEVELOPMENT OF SEISMIC RESISTANT HIGH-STRENGTH LOW-CARBON DUAL-PHASE STEEL PLATE WITH GOOD LOW-TEMPERATURE TOUGHNESS

P26

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Dual-phase steels have a composite microstructure in which a hard second phase (martensite) is dispersed in a soft ferrite matrix. This composite microstructure of dual-phase steels provides interesting and excellent mechanical properties such as good ductility, high rate of work hardening, low yield-to-tensile ratio, and continuous yielding behavior which offer advantages compared with conventional high-strength low alloy steels. Given that the mechanical properties of dual-phase steels depend strongly on microstructure factors such as grain size, morphology, and volume fraction, it is necessary to optimize the microstructure factors through a suitable selection of chemical composition and heat treatment conditions. As several microstructure factors interact with each other and often change simultaneously rather than independently, however, a systemic understanding of their effect on the mechanical properties of dual-phase steel is essential. In this study, high-strength low-carbon dual-phase steels with different microstructure factors were fabricated by controlling chemical composition and intercritical annealing conditions after direct quenching following austenitizing. Based on the SEM, EBSD, TEM, and Thermocalc-DICTRA simulation, microstructural evolution during intercritical annealing was discussed. In addition, tensile and Charpy V-notch impact tests were conducted at various temperatures to investigate the correlation between the microstructure factors and the mechanical properties for the development of seismic resistant high-strength low carbon dual-phase steels with good low-temperature toughness.

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EFFECT OF SI CONTENT ON HYDROGEN EMBRITTLEMENT OF TEMPERED MARTENSITIC STEELS

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The effect of Si content on the microstructure, tensile property and hydrogen embrittlement (HE) resistance of tempered martensitic steels was investigated in this study. Film-like cementite formed along grain boundaries was strongly suppressed with increasing Si content, resulting in the preferred formation of short rod-like cementite. The tensile and fracture behaviors of tempered martensitic steels with different Si content were evaluated by using a slow strain-rate tensile test after hydrogen charging. Increasing Si content enhanced the HE resistance characterized by relative reduction of area. To elucidate the beneficial effect of Si addition, thermal desorption spectroscopy (TDS), silver decoration and fractography analysis were conducted on the hydrogen pre-charged steel specimens. The decreased fraction of film-like cementite improved the HE resistance because the interface between film-like cementite and matrix acts as reversible trapping sites for hydrogen. This was supported by the decrease in the concentration of diffusible hydrogen measured by TDS.

INFLUENCE OF CARBIDE TYPES ON THE HIGH-TEMPERATURE OXIDATION KINETICS OF HOT-WORK TOOL STEELS

P28

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The influence of carbide types on the high-temperature oxidation kinetics of three hot-work tool steels was investigated in two conditions, the soft annealed condition, and the quenched and tempered condition. Two of the steels studied are classified as chromium hot-work steels (AISI H11 and Dievar) and the third cannot be classified using the AISI classification for hot-work steels as it is a newly developed steel with increased thermal conductivity (W600). The first two are well known and studied and contain mainly chromium and molybdenum-based carbides ($M_{23}C_6$, M_7C_3, M_6C and M_2C) and some vanadium-based carbides (MC). The third one, on the other hand, contains mainly molybdenum- and tungsten-based carbides (M_6C and MC). Initial calculations of the thermodynamically stable equilibrium phases as a function of temperature were carried out using the CALPHAD method. The kinetics were investigated in dry air with a simultaneous thermal analyser (STA) using the thermogravimetric analysis method (TGA). The temperature range was between 400 °C and 700 °C and the oxidation time was 100 hours. It was found that chromium-based carbides in particular affect the oxidation kinetics, which is shown as a fluctuation in the TGA curves, but only at lower temperatures (< 600 °C), as diffusion is slower and wüstite is thermodynamically unstable up to 570 °C. At higher temperatures, chromium-based carbides do not have a strong influence on the oxidation kinetics, while molybdenum- and tungsten-based carbides do not have a major influence on the kinetics at any of the temperatures studied. As for the condition of the steels, the steels in the soft annealed condition generally show less fluctuations in the TGA curves, which is due to the large spherical carbides. It has been shown that oxidation is more continuous with larger or coarser carbides and consequently the oxide layer formed is thicker. This means that the larger the carbides, the greater the influence on the oxidation kinetics. This was also confirmed by the TGA results. When we compare two states based on the alloying elements dissolved in the matrix, steels in the quenched and tempered state oxidise less than those in the soft annealed state.

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TEMPERATURE GRADIENTS FOR DATA MINING

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Industrial R&D departments and also academic research facilities appear to be more and more pressed for time when working on improvement of existing materials or developing new materials. Computer simulations may be employed to support experimental efforts, but they heavily depend on reliable material data. Similarly, the design of components requires detailed knowledge about material properties. It is evident that the availability of comprehensive data bases accelerates material development efforts. However, for many material classes, data bases are incomplete, contain estimations or extrapolations, or are in the worst case non-existent.

One of the goals of research in materials science should thus be to provide the necessary data. However, conventional 'data mining' is often tedious, requiring waiting times for thermal equilibrium or steady states to be achieved. The development of high-throughput methods is one of the pathways to larger data bases that contain data on pure substances and also binary and multicomponent alloys. Automated production and evaluation of a series of compositions or thermodynamic states of alloys is certainly a viable way to improve the availability of data.

Methods for efficient data mining that are at present being developed at FSU Jena are based on graded samples. Temperature gradients are used to create concentration gradients, and the changes of properties with concentration and temperature are evaluated with state-of-the-art experimental and numerical methods. The state of the research is such that the methods can be accessible for pertinent research labs. With respect to the synthesis of the appropriate graded samples, distinct development steps have been achieved recently. The potential of the evaluation of such samples is demonstrated for thermodynamic data (solidus and liquidus lines/surfaces, among others), kinetic data (frequency factors and activation energies of diffusion coefficients) and thermal data (thermal diffusivity, thermal conductivity and heat capacity).

FACTSAGE EQUILIBRIA SIMULATIONS AS A TOOL TO ENVISAGE CORROSION OF REFRACTORY MATERIALS FOR THE COPPER INDUSTRY

P30

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Copper is a key raw material both in Poland and worldwide. It ensures economic growth and civilizational development. In 2020, Poland was 7. the biggest producer of smelted copper. 75 % out of total Cu demand (30 mln t/year) is applied in electric energy production. In recent years, we observe a dynamic increase in the Cu demand. In the last 20 years, annual demand for copper has doubled, and the forecast shows that the demand will be doubled again by 2030. This is driven by the development of green energy installations, and elements of electric vehicles as, e.g., the electric car contains four times more Cu (83 kg) than traditional combustion-engine vehicles.

Refractory materials are indispensable for the production of copper. Corrosion is one of the most significant factors which influence the accelerated consumption of refractory materials. An aggressive chemical environment and high-temperature conditions up to 1350°C enhance interactions between components of refractory and copper slag/copper/alloy. As the development of new refractories requires a long, complex and costly process starting from design, production, and experimental testing, the application of computer programs equipped with thermochemical databases can efficiently shorter this path, via predicting the high-temperature reactions.

In this work, we present the application of selected modes of FactSage equilibria software (coupled with databases covering liquid Cu, slags and oxide solid solutions) to predict high-temperature reactions between Cr-containing and Cr-free refractory material. Also, alternations in phase compositions of copper slags were calculated and validated experimentally. Based on the results, we show how the application of such thermodynamic software can support scientist/refractory materials technologists by fostering the high-temperature phenomena in a complex environment, thus, limiting the number of experiments, reducing the costly the B+R process, and making it more sustainable.

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HOW FACTSAGE SOFTWARE CAN FACILITATE WORK IN REFRACTORY MATERIALS SCIENCE

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Refractory materials are indispensable for the production of steel, non-ferrous metals like copper or lead, cement, glass, ceramics, and numerous other materials. In the process of designing new refractory materials/optimization of existing refractories, or testing their corrosion, utilization of FACTSAGE software equipped with thermochemical databases is very useful, as it allows more effective development of new or modified refractory materials.

FactSage is thermochemical software that is fully integrated with multiple databases. It includes various modules and permits for different thermodynamic calculations, in an equilibria state. The 'Reaction' module of FactSage allows the calculation of changes in extensive thermochemical properties: activity, C_p, H, G, V and S for a single or a mixture of species reacting with each other at a specific temperature. The 'Equilib' module of FactSage, by using algorithms based on the global Gibbs energy minimization, provides information about the equilibrium state of a heterogenous system defined by chemical composition, pressure and temperature. The 'Viscosity' module can calculate the change of the viscosity of liquid slag depending on its actual chemical composition *vs.* temperature.

In this work, we demonstrate the application of various modes of FactSage software, including Equilib, Reaction and Viscosity, in refractory materials science as a tool that greatly facilitates laboratory work as well as shortens the process of designing the new innovative refractories. Numerous systems concerning refractory materials and slags occurring in the copper industry were analyzed and presented.

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TOFA 2024

19th Discussion Meeting on Thermodynamics of Alloys

THERMODYNAMICS of ALLOYS

Fall 2024
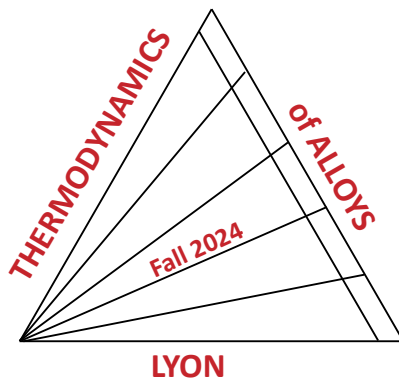
LYON

The 19th Discussion Meeting on Thermodynamics of Alloys will take place in Lyon, France in the fall of 2024. Lyon is the second-largest metropolitan area of France. It is located at the confluence of the rivers Rhone and Saone, 391 km (243 mi) southeast of Paris, 278 km (173 mi) north of Marseille, 113 km (70 mi) southwest of Geneva. The capital of the Gauls during the Roman Empire, Lyon became a major economic hub during the Renaissance. The city is recognised for its cuisine and gastronomy, as well as historical and architectural landmarks; as such, the districts of Old Lyon, the Fourvière hill, the Presqu'ile and the slopes of the Croix-Rousse are inscribed on the UNESCO World Heritage List. Lyon was historically an important area for the production and weaving of silk. Lyon played a significant role in the history of cinema since Auguste and Louis Lumière invented the cinematograph there. The city is also known for its light festival, the Fête des Lumières, which begins every 8 December and lasts for four days, earning Lyon the title of "Capital of Lights".

The home of three renowned universities and several higher education schools, Lyon is the second-largest student city in France, with a university population of nearly 200,000 students within the Metropolis of Lyon.

As usual TOFA 2024 will be an opportunity for all generations to meet. Researchers, scientists and students in the field of thermodynamics of alloys are welcome to join this international conference.

Olivier DEZELLUS – Chair of TOFA 2024

Conference topics include, but are not limited to:

- Experimental and theoretical thermodynamics – new results and techniques
- Computational thermodynamics
- Thermodynamic properties derived from ab initio calculations
- Phase diagrams
- Phase transformations and kinetics, solid state diffusion
- Thermodynamics of low-dimensional systems (surfaces and interfaces, nanomaterials)
- Thermochemistry of metallurgical processes
- Process simulation using thermodynamics
- Industrial applications of thermodynamics

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