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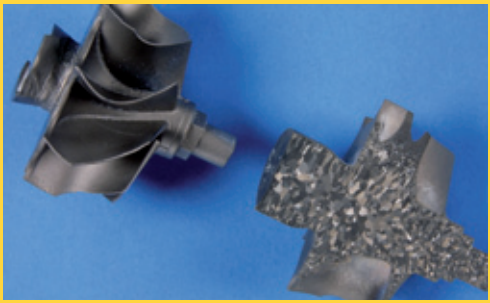
PROGRAMME AND ABSTRACTS

Intermetallics 2015




International Conference

28 September – 02 October 2015

Educational Center Kloster Banz • Germany

www.intermetallics-conference.de

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Dear Colleagues and Friends,

Following the first successful conference in this series, it is again our pleasure to welcome you to the Intermetallics 2015 Conference at the Educational Center Kloster Banz, Germany.

Facing an increasing demand for new materials with improved properties, intermetallic-based materials offer a promising perspective. A possible combination of high strength, low density and good corrosion resistance qualifies them for structural applications, specifically at high temperatures and in severe environments. As some intermetallic phases show unique properties like shape memory and thermo electric effects or have appealing magnetic properties they are also of interest for various functional applications. With the advent of new generations of aeroengines they are finally – after three decades of exhaustive research and development – also used for structural applications.

The choice of local organisers and members of the international advisory board has brought together a total number of 116 presentations spanning from fundamental research towards application-oriented subjects. Following the successful format established during the first Intermetallics conference, again topics of general importance will be presented in a single session in the morning, while more specialized information on different material classes, such as titanium, iron and nickel aluminides, silicides, or certain aspects of intermetallics will be the subject of two specialised parallel sessions in the afternoon. This event's special topical session is devoted to the application of computational thermodynamics to intermetallic materials. A high-profile poster session rounds off the conference.

The conference again takes place at Kloster Banz near Bamberg. As the cloister is situated in a remote place above the valley of the river Main, we believe this to be the ideal place for conferences with its good infrastructure and relaxing atmosphere.

We are delighted to welcome you in Kloster Banz,

Your Intermetallics 2015 Organising Team

Venue and date
Educational Center Kloster Banz
Hanns-Seidel-Stiftung e. V. • 96231 Bad Staffelstein (DE)
28 September–02 October 2015

Scientific organiser
Martin Heilmaier, Karlsruhe Institute of Technology, Karlsruhe

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Registration fees

Student		250 EUR
University/Institute		500 EUR
Industry		700 EUR
Accompanying Person*		250 EUR
Workshop: School on Thermodynamics of Intermetallics**		included

Social programme***

Get together	28 September 2015	included
Conference dinner	30 September 2015	included
Excursion • Hiking tour	01 October 2015	6 EUR
Excursion • Bus tour	01 October 2015	20 EUR

* Get together and Conference dinner is included.

** Number of participants limited and only for students.

*** Registration for the Social programme is required.

General terms and conditions

Please find our General Terms and Conditions at www.intermetallics-conference.de.

Opening hours	**Monday**	**Thursday**	**Wednesday**	**Thursday**	**Friday**
Check-In	08^{00}–20^{00}	08^{30}–16^{30}	08^{30}–16^{30}	08^{30}–14^{00}	08^{30}–13^{00}

Internet

Voucher for Wireless-Lan are available at the registration desk from the Kloster Banz.

Certificate of attendance

Certificates of attendance will first be made available on the last day of the conference at the check-in desk.

Poster prizes

The three best posters will be awarded with 300 EUR.

Poster Session
Posters will be rated on Tuesday, 29 September 2015, 19:00. Authors are requested to be present at their posters during the poster session.

Drinks and finger food will be served during the poster session.

Pinboards will be numbered. The pinboards are only to be used with the designated pins. You will find your poster number in the programme book on page 24.

Please note that all posters should be hanging on Tuesday, 29 September 2015, by 16:00 and be removed at the latest by Friday, 2 October 2015, 11:00. Posters that have not been removed by that time will be considered as waste.

Catering
Foods and drinks during the breaks will be provided.

The restaurant "Klosterschänke" is directly located on the premises of Kloster Banz and is open daily from 10:00–22:00.

For your information: the closest city with alternative restaurants is Bad Staffelstein, which is 5.5 km away (approximately 1 hour by foot, 7 minutes by car).

Media cooperation
We would like to thank the following partners for their great support for the Intermetallics 2015 conference.
Carl Hanser Verlag GmbH & Co. KG (Munich/DE)
"International Journal of Materials Research"
"Praktische Metallographie"

Smoking
Smoking is prohibited inside the entire conference centre.

Taxi • Taxi Dütsch

Phone	+49 9573 52 06/+49 9571 52 06
Price from Bad Staffelstein to Kloster Banz	about 10 EUR*
Price form Lichtenfels to Kloster Banz	about 13 EUR*

* Prices are subject to change.

Submitting your presentation/technical information
Please prepare your presentation as PDF, MS Office PowerPoint2007, 2010 for Windows or key for Macintosh DVD in 4:3 aspect ratio.

A presentation notebook with a PDF reader and MS Office PowerPoint 2010/2007 will be provided. Notebook, presenter and laser pointer will be available at the speaker's podium in the lecture hall. The use of personal notebooks is possible upon agreement. However, it may interrupt the flow of the programme in the lecture hall. You will be assisted by a technical supervisor.

To guarantee a smooth running programme please upload your presentation on time – at least 2 hours before your presentation starts.

For submission, please use a USB flash drive, CD or DVD disc that is not protected by any software. Professional staff and equipment will be available for you to arrange and preview your presentation.
Please note: certain encodings for video and audio files could lead to technical problems.

Time Allotment
Please prepare your presentation for the allotted amount of time. Chairs and moderators may interrupt should you overrun your time limit.

Allotted time is assigned as follows (speaking + discussion time):

1. Invited talk	20 + 5 minutes discussion
2. All other single-session and parallel session talks	15 + 5 minutes discussion

Get together* • Monday, 28 September 2015
Come together for drinks and snacks. Enjoy the evening and allow yourself interesting conversations with colleagues, old friends and new acquaintances.

18:30	Welcome
20:00	Opening
20:30	Opening talk • Novel Design Principles using TCP Phases in Austenitic Heat Resistant Materials Masao Takeyama (Tokyo/Japan)

Conference dinner* • Wednesday, 30 September 2015
Take the chance to get in touch with friends and colleagues and have an enjoyable evening. The conference dinner starts with the award of the poster prizes.

Start	19:00 in the "Kaiser Saal"
Fee	included

Excursion* • Thursday, 01 October 2015
You can choose between hiking tour Vierzehnheiligen or a bus tour to Nuremberg with a guided tour through the "Albrecht-Dürer-House" in English.

Hiking tour Vierzehnheiligen

Start	14:00 at Kloster Banz (car park)
Duration	5,5 h
Fee	6 EUR

Please make sure to wear appropriate footwear. At 19:30 the bus returns back to Kloster Banz.

Bus tour Nuremberg with guided tour

Start	14:00 at Kloster Banz (car park)
Duration	6 h
Fee	20 EUR (incl. guided tour)

A guided tour through the "Albrecht-Dürer-House" is included. After the guided tour you can use your free time (16:30–20:00) to explore the city of Nuremberg with all their cultural attractions by yourself. At 20:00 the bus returns back to Kloster Banz.

** A registration is necessary.*

Monday, 28.09.2015 School on Thermodynamics of Intermetallics*	Tuesday, 29.09.2015		Wednesday, 30.09.2015		Thursday, 1.10.2015		Friday, 2.10.2015
Seminar room 6	Main hall	Seminar room 6	Main hall	Seminar room 6	Main hall	Seminar room 6	Main hall
09:00–10:30	09:00–10:30		09:00–10:30		09:00–10:30		09:00–10:30
Phase diagrams and phase transformations P. 10	Invited talks and Talks 1 P. 12		Invited talks and Talks 3 P. 17		Invited talks and Talks 5 P. 21		Invited talks and Talks 6 P. 23
Coffee break	*Coffee break*		*Coffee break*		*Coffee break*		*Coffee break*
11:00–12:30	11:00–12:30		11:00–12:30		11:00–12:20	11:00–12:20	11:00–12:20
Key experiments and experimental techniques P. 10	Invited talks and Talks 2 P. 13		Invited talks and Talks 4 P. 17		Session Ti aluminides 4 P. 21	Session Special topic P. 22	Session Miscellaneous and Ti aluminides 5 P. 23
Lunch	*Lunch*		*Lunch*		*Lunch*		*Lunch*
14:00–15:30	14:00–16:00	14:00–16:00	14:00–16:00	14:00–16:00	14:00–20:00		
Thermodynamic modelling (CALPHAD) of phase diagrams P. 11	Session Ti aluminides 1 P. 13	Session Ni aluminides and Superalloys P. 14	Session Ti aluminides 2 P. 18	Session Fe aluminides 2 P. 19			
Coffee break	*Coffee break*		*Coffee break*				
16:00–17:30	16:30–18:30	16:30–18:30	16:30–18:30	16:30–18:30			
Ab initio calculations for materials design P. 11	Session Fe aluminides 1 P. 15	Session Functional intermetallics and Miscellaneous P. 15	Session Ti aluminides 3 P. 19	Session Silicides P. 20	Excursion/Hike P. 8		
Main hall							
18:30							
Get together with Opening and Opening talk P. 12	19:00-21:00 Postersession P. 24		19:00-23:00 Conference dinner and Awards P. 8				

* The school is especially intended for students and young scientists, the possible number of participants is limited. A registration is necessary. There are no additional costs.

09:00–17:30 **School on Thermodynamics of Intermetallics**

Seminar room 6

09:00–10:30 Phase diagrams and phase transformations
Frank Stein (Düsseldorf/DE)

Phase diagrams are the basis for any materials development. They contain information not only about phase equilibria and about the occurrence of phase transformations for a material of any chemical composition. By additionally having some knowledge about the kinetics of possibly involved phase transformations, phase diagrams also tell us a lot about the microstructure of a material with a certain chemical composition, which in turn already allows concluding on the mechanical properties to be expected for this material. The primary objective of the lecture will be to show how phase diagrams can be used and which information can be read from them.

10:30–11:00 *Coffee break*

11:00–12:30 Key experiments and experimental techniques
Martin Palm (Düsseldorf/DE)

Quite a number of experimental techniques exist for the determination of phase equilibria and phase transitions. Metallography, quantitative chemical analysis of phases by energy or wavelength dispersive spectrometry (EDS, WDS), X-ray diffraction (XRD) or differential thermal analysis (DTA) are some of them. In addition, a proper heat treatment is necessary to attain and preserve thermodynamic equilibrium. The capabilities of these techniques will be briefly introduced. Discussion will focus on practical aspects, e.g. how to decide whether a sample is in thermodynamic equilibrium and how the quality of individual data can be judged.

12:30–14:00 *Lunch*

14:00–15:30 Thermodynamic modelling (CALPHAD) of phase diagrams
Aleš Kroupa (Brno/CZ)

The theoretical modelling of phase diagrams has become a key tool in the development of new materials and improvement of material properties of existing ones. The most applicable theoretical method for modelling of phase diagrams is the semiempirical CALPHAD method. The method can be used for very complex alloys, corresponding to real materials, and allows us to decrease significantly the extent of experimental work. We can test theoretically a large number of compositions in the search for materials with favorable properties. The CALPHAD method is currently the most widely used for the applications in basic and applied research and in materials development in industry. The basic principles of the CALPHAD methods will be described in the lecture, together with examples of its application, strengths and weaknesses, its prediction capabilities etc. Also the basic information about existing software packages, thermodynamic databases and rules for their development will be mentioned here.

15:30–16:00 *Coffee break*

16:00–17:30 *Ab initio* calculations for materials design
Martin Friák (Brno/CZ)

Quantum-mechanical (so-called ab *initio*) methods have recently achieved considerable reliability when predicting materials properties. *Ab initio* calculations provide a deeper insight and understanding of matter at the atomic scale with an unprecedented level of detail and accuracy. Owing to their universality and reliability, they are becoming increasingly useful not only when studying existing materials but also when designing new ones. Importantly, whenever experimental data are missing, quantum-mechanical calculations represent a unique source of information for other modeling approaches, e.g., semiempirical thermodynamic calculations of phase diagrams (CALPHAD), atomistic and continuum methods, or multi-scale materials simulations. The quality of the *ab initio* description is not limited to ground-state parameters – material responses to rather extreme external conditions can reliably be determined as well. The lecture will (i) exemplify the use of *ab initio* calculations in current computational materials science, (ii) overview available software tools, (iii) identify major challenges, and (iv) outline a few foreseen future trends.

Scientific programme • Monday, 28 September 2015

18:30–21:00	**Get together** (in front of main hall)
20:00–20:15 Main hall	Opening Martin Heilmaier (Karlsruhe/DE)
20:15–21:00 Main hall	Opening Talk Novel Design Principles using TCP Phases in Austenitic Heat Resistant Materials Masao Takeyama (Tokyo/JP)

Scientific programme • Tuesday, 29 September 2015

09:00–10:30 Main hall	**Invited talks and Talks 1** Chair: Janny Lindemann (Freiberg/DE)
09:00 O–IT 02	**Invited talk**: TiAl alloy technology trends and future opportunities in aircraft engines Bernhard P. Bewlay (Niskayuna, New York/US)
09:25 O–IT 03	**Invited talk**: Fatigue strength in γ-TiAl produced by additive manufacturing – a few lessons learnt Mauro Filippini (Milano/IT)
09:50 O–TA 01	Formation of a fine and resistant microstructure in TiAl alloys by spark plasma sintering Alain Couret (Toulouse/FR)
10:10 O–TA 02	TiAl revert conversion into feed stocks for the production of aircraft engine components Volker Güther (Nuremberg/DE)
10:30–11:00	*Coffee break*

11:00–12:30	**Invited talks and Talks 2**
Main hall	Chair: Martin Friák (Brno/CZ)
11:00	**Invited talk**: *Ab-initio* based assessment of the thermodynamic
O–IT 04	stability of Al-based intermetallic phases
	Tilmann Hickel (Düsseldorf/DE)
11:25	**Invited talk**: Effective cluster interactions and intermetallics
O–IT 05	thermodynamics
	Claudio Schön (São Paulo/BR)
11:50	Al-Fe-Ni-Ti Calphad state of the art
O–ST 01	Nathalie Dupin (Orcet/FR)
12:10	Thermodynamic study of the Nb-Ru-Al ternary system:
O–ST 02	experimental and Calphad approaches
	Michel Vilasi (VAndoeuvre les Nancy/FR)
12:30–14:00	*Lunch*
	Parallel sessions
14:00–16:00	**Session Ti aluminides 1**
Main hall	Chairs: Volker Güther (Nuremberg/DE)
	Bernhard P. Bewlay (Niskayuna, New York/US)
14:00	Manufacturing and properties of TiAl TNM® sheet materials
O–TA 03	Janny Lindemann (Freiberg/DE)
14:20	High-speed die forging of TiAl alloy
O–TA 04	Keiji Kubushiro (Yokohama/JP)
14:40	*In situ* synchrotron radiation study during hot forming of a
O–TA 05	Nb-rich TiAl alloy
	Andreas Stark (Geesthacht/DE)
15:00	A new processing route for forged TiAl automotive engine valves
O–TA 06	Dong Liu (Shenyang/CN)

15:20 O–TA 07 — Microstructure and texture characteristics of extruded Ti-47Al-2Cr-2Nb-0.15B with different initial microstructure of billets
Renci Liu (Shenyang/CN)

15:40 O–TA 08 — Microstructure formation and phase composition in diffusion brazed γ-TiAl-alloy joints
Katja Hauschildt (Geesthacht/DE)

14:00–16:00 Session Ni aluminides and Superalloys
Seminar room 6 Chairs: Easo George (Bochum/DE)
Werner Skrotzki (Dresden/DE)

14:00 O–NA 01 — The influence of the Al-concentration on the fracture toughness, hardness and Young's modulus of NiAl single crystals
Steffen Neumeier (Erlangen/DE)

14:20 O–NA 02 — Influence of microstructure on the oxidation behavior of directional solidified eutectic NiAl-X (X = Cr, Mo)
Ioannis Sprenger (Karlsruhe/DE)

14:40 O–NA 03 — Study of the hot workability of the directionally solidified fibre-reinforced NiAl-W eutectic alloy
Arcadio Varona-Caballero (Getafe, Madrid/ES)

15:00 O–NA 04 — Micromechanical investigation of the deformation of NiAl-Cr directionally solidified eutectic alloys
Amritesh Kumar (Eggenstein-Leopoldshafen/DE)

15:20 O–SA 01 — Physical simulation of investment casting of nozzle guide vanes made of Ni-based superalloys
Mehdi Rahimian (Getafe, Madrid/ES)

15:40 O–SA 02 — Orientation relationships and phases in Co-Al-W alloys
Nataliya Kazantseva (Ekaterinburg/RU)

16:00–16:30 Coffee break

Parallel sessions

16:30–18:30	**Session Fe aluminides 1**
Main hall	Chairs: Elzbieta Godlewska (Krakow/PL) Saeid Lotfian (Düsseldorf/DE)
16:30 O–FA 01	Microstructure refinement in iron aluminide based alloys through industrial processing Martin Palm (Düsseldorf/DE)
16:50 O–FA 02	Hierarchical microstructure of ferritic superalloys Christian Liebscher (Düsseldorf,Berkeley/DE,US)
17:10 O–FA 03	Effect of ordering on the fracture toughness and creep resistance of Fe-Al-Nb alloys Srdjan Milenkovic (Madrid/ES)
17:30 O–FA 04	Influence of B on structure and mechanical properties of Fe-Al-Nb intermetallic alloys Alena Michalcova (Düsseldorf/DE)
17:50 O–FA 05	Morphology of Fe-Al intermetallic layers evolving in a spark plasma sintering apparatus Hanka Becker (Freiberg/DE)
18:10 O–FA 06	Intermetallic compounds as catalysts for the semi-hydrogenation of acetylene Marc Armbrüster (Chemnitz/DE)
16:30–18:30	**Session Functional intermetallics and Miscellaneous**
Seminar room 6	Chairs: Kiyohito Ishida (Sendai/JP) Claudio Schön (São Paulo/BR)
16:30 O–FU 01	Temperature dependence of mechanical properties of the $Fe_{81}Ga_{19}$ (Galfenol) alloy Shien-Uang Jen (Taipei/TW)
16:50 O–FU 02	The nano-crystalline superelastic NiTi intermetallic – the effect of heat treatment on the structural, mechanical and corrosion characteristics Jiří Kubásek (Prague/CZ)

17:10 O–FU 03	Correlation between electrical resistivity and phase intermetallic structure in the 3D porous SMA synthesized during SLS/M process Igor Shishkovsky (Samara/RU)
17:30 O–FU 04	Ferromagnetic shape memory alloys Jaromír Kopeček (Prague/CZ)
17:50 O–MI 01	Growth of stoichiometric intermetallic phases as single phase in a temperature gradient Stephanie Lippmann (Jena/DE)
18:10 O–MI 02	The effects of thermo-mechanical treatments on the microstructure and mechanical properties of AFA steels Bin Hu (Hanover/US)
19:00	*Poster session at foyer with snacks and drinks*

09:00–10:30 Main hall	**Invited talks and Talks 3** Chair: Frank Stein (Düsseldorf/DE)
09:00 O–IT 06	**Invited talk**: Phase stability and mechanical properties of high-entropy alloys Easo George (Bochum/DE)
09:25 O–IT 07	**Invited talk**: Combinatorial materials research for novel intermetallic alloy systems Alfred Ludwig (Bochum/DE)
09:50 O–FU 05	Phase stability of intermetallic compound in Cu-Mn-Al and Cu-Ni-Al alloys and industrial applications Kiyohito Ishida (Sendai/JP)
10:10 O–MI 03	NMR as a local probe for intermetallics Frank Haarmann (Aachen/DE)
10:30–11:00	*Coffee break*
11:00–12:30 Main hall	**Invited talks and Talks 4** Chair: Manja Krüger (Magdeburg/DE)
11:00 O–IT 08	**Invited talk**: High temperature Mo-Si-B alloys – phase stability and environmental resistance John Perepezko (Madison, Wisconsin/US)
11:25 O–IT 09	**Invited talk**: Application of chevron-notched micro-size fracture testing method on single crystal Si and Nb-Si intermetallic compound Seiji Miura (Sapporo/JP)
11:50 O–ST 03	High entropy silicide composites? – What are the rules for designing their high entropy solid solution phase? Panagiotis Tsakiropoulos (Sheffield/UK)
12:10 O–SI 01	Environmental/thermal barrier coating systems for Nb/Nb_5Si_3-based high-temperature alloys Reinhold Braun (Köln/DE)
12:30–14:00	*Lunch*

Parallel sessions

14:00–16:00 Main hall

Session Ti aluminides 2

Chairs: Michael Oehring (Geesthacht/DE)
Jose San Juan (Bilbao/ES)

14:00 O–TA 09
Large scale forging of an advanced Ti-Al-Nb alloy
Marcus Rackel (Geesthacht/DE)

14:20 O–TA 10
Measuring plastic deformation of titanium aluminides under compressive and tensile uniaxial loading using sub-micron resolution digital image correlation and Kikuchi diffraction mapping
Thomas Edward James Edwards (Cambridge/UK)

14:40 O–TA 11
Describing the temperature-dependent yield point of polysynthetically twinned TiAl crystals by means of a thermomechanically coupled crystal plasticity model
Jan Eike Butzke (Geesthacht/DE)

15:00 O–TA 12
Segregation of C and Si in lamellar microstructures of β-solidifying γ-TiAl-Based Alloys
Thomas Klein (Leoben/AT)

15:20 O–TA 13
Carbides in γ-TiAl alloys with varying alloying elements and thermal history
Florian Pyczak (Geesthacht/DE)

15:40 O–TA 14
Influence of niobium, tantalum and zirconium on lattice parameter and hardness of the α_2- and γ-phase in fully lamellar titanium aluminides
Johannes Bresler (Erlangen/DE)

14:00–16:00 **Session Fe aluminides 2**
Seminar room 6 Chairs: Srdjan Milenkovic (Madrid/ES)
Alena Michalcova (Düsseldorf/DE)

14:00 Iron aluminide alloys modified with selected ternary additions
O–FA 07 Elzbieta Godlewska (Krakow/PL)

14:20 Coarsening kinetics of lamellar FeAl + $FeAl_2$ microstructures in
O–FA 08 Al-rich Fe-Al alloys
Xiaolin Li (Düsseldorf/DE)

14:40 Creep properties and microstructure of binary Fe-Al alloys
O–FA 09 with a fine-scaled, lamellar microstructure
Martin Heilmaier (Karlsruhe/DE)

15:00 Chemically graded iron aluminide – steel samples fabricated by
O–FA 10 laser metal deposition (LMD)
Saeid Lotfian (Düsseldorf/DE)

15:20 Comparison of high temperature oxidation of Fe-40Al coatings
O–FA 11 obtained by CGS and HVOF
Núria Cinca (Barcelona/ES)

15:40 Comparison of thermal sprayed coatings from iron aluminide
O–FA 12 powders deposited by HVOF, plasma and flame spray techniques on an Al-Si-alloy
Philipp Gerhard Thiem (Magdeburg/DE)

16:00–16:30 *Coffee break*

Parallel sessions
16:30–18:30 **Session Ti aluminides 3**
Main hall Chairs: Mauro Filippini (Milano/IT)
Alain Couret (Toulouse/FR)

16:30 The influence of aerofoil structure on metallurgical quality of
O–TA 15 cast TiAl turbine blades
Rui Yang (Shenyang/CN)

16:50 Columnar-to-equiaxed transition and peritectic solidification
O–TA 16 in γ TiAl alloys
Nicole Reilly (Nancy/Colombes/FR)

17:10 O–TA 17	Influence of borides on the phase transformation kinetics in γ titanium aluminide alloys Michael Oehring (Geesthacht/DE)
17:30 O–TA 18	Centrifugal investment casting of γ TiAl automotive engine pistons Yuyou Cui (Shenyang/CN)
17:50 O–TA 19	*In-situ* study of the time-temperature-transformation behaviour of an intermetallic γ-TiAl based alloy Petra Erdely (Leoben/AT)
18:10 O–TA 20	Atomic relaxation processes at high temperature in Mo-rich β/γ-Ti-Al intermetallics Jose San Juan (Bilbao/ES)

16:30–18:30 **Session Silicides**
Seminar room 6 Chairs: John Perepezko (Madison/US)
Martin Heilmaier (Karlsruhe/DE)

16:30 O–SI 02	Determining the eutectic point of Mo-rich Mo-Si-B alloys Georg Hasemann (Magdeburg/DE)
16:50 O–SI 03	Directional solidification of ternary Nb-Si-Cr eutectics and its influence on the creep behavior Florian Gang (Karlsruhe/DE)
17:10 O–SI 04	Interface structures in directionally solidified $MoSi_2/Mo_5Si_3$/ Mo_5Si_3C eutectic composites Hirotaka Matsunoshita (Kyoto/JP)
17:30 O–SI 05	Bond coat alumina forming intermetallic alloys for coatings for Nb silicide alloys Panagiotis Tsakiropoulos (Sheffield/UK)
17:50 O–SI 06	The oxidation behaviour and crystallographic features of single phased $(TT'Cr)_7Si_6$ silicides (with T = Nb and Ti and T' = Fe, Co, Ni) Michel Vilasi (Vandoeuvre lès Nancy/FR)
18:10 O–SI 07	Effect of Si concentration on the properties of V-Si solid solution powders Janett Schmelzer (Magdeburg/DE)

19:00–23:00 *Conference dinner (see page 8)*

09:00–10:30	**Invited talks and Talks 5**
Main hall	Chair: Masao Takeyama (Tokyo/JP)
09:00 O–IT 10	**Invited talk**: Effects of vacancy-site occupation on phase stability, thermoelectric properties, and mechanical behavior of half-Heusler MNiSn (M: Ti, Zr, Hf) alloys Yoshisato Kimura (Yokohama/JP)
09:25 O–IT 11	**Invited talk**: Synergies between theoretical and experimental methods in modern materials science – an insight from *ab initio* calculations Martin Friák (Brno, Düsseldorf/CZ, DE)
09:50 O–ST 07	Supersaturated intermetallic phases within the ternary Mo-Cr-N system Paul Mayrhofer (Vienna/AT)
10:10 O–MI 04	Intermetallic precipitates in cobalt-free, low alloyed secondary hardening steels Alexander Zimmermann (Aachen/DE)
10:30–11:00	*Coffee break*
	Parallel sessions
11:00–12:20	**Session Ti aluminides 4**
Main hall	Chair: Núria Cinca (Barcelona/ES)
11:00 O–TA 21	Stability issues at the boundary between *in-situ* grown oxides on selective halogenated intermetallic titanium aluminides Raluca Pflumm (Frankfurt am Main/DE)
11:20 O–TA 22	Investigation on the absorption of fluorine in γ-TiAl and it simpact on the oxidation behavior and microstructure Peter Spiess (Aachen/DE)
11:40 O–TA 23	Oxidation behaviour of γ-TiAl alloys coated with intermetallic Ti-Al-Cr based layers Nadine Laska (Köln/DE)

12:00 O–TA 24	TEM studies of the uncoated and coated Ti-46Al-8Nb specimens after a long-term exposure to air at 700°C Elzbieta Godlewska (Krakow/PL)
11:00–12:20 Seminar room 6	**Session Special Topic** Chair: Nathalie Dupin (Orcet/FR)
11:00 O–ST 04	Interactions of liquid Au-Si with Cu, Ni and Ti – phase equilibria and new ternary compounds Klaus W. Richter (Vienna/AT)
11:20 O–ST 05	Modelling topologically close-packed phases in superalloys and steels Thomas Hammerschmidt (Bochum/DE)
11:40 O–ST 06	Thermodynamic modelling at low temperatures – combined *ab initio*, semiempirical and experimental approach Jana Pavlů (Brno/CZ)
12:00 O–ST 08	*Ab initio* study on stacking faults in γ-TiAl Philip Dumitraschkewitz (Leoben/AT)
12:20–14:00	*Lunch*
14:00–20:00	Hiking tour Vierzehnheiligen
14:00–21:00	Bus tour Nuremberg

09:00–10:30 Main hall	**Invited talks and Talks 6** Chair: Yoshisato Kimura (Yokohama/JP)
09:00 O–IT 12	**Invited talk**: Nickel-titanium-hafnium alloys with high strength and advanced functional performances Aaron Stebner (Golden/US)
09:25 O–IT 13	**Invited talk**: Mechanical properties of novel polycrystalline Co-base superalloys with $L1_2$ ordered precipitates Steffen Neumeier (Erlangen/DE)
09:50 O–SA 03	Effect of ordering on hydrogen affected dislocation behavior in Ni-Cr superalloys Kaori Kawano (Amagasaki, Hyogo/JP)
10:10 O–MI 05	Diffusion in binary silicides of iron and molybdenum Helmut Mehrer (Obersteinenberg/DE)
10:30–11:00	*Coffeebreak*
11:00–12:20 Main hall	**Session Miscellaneous and Ti aluminides 5** Chair: Martin Palm (Düsseldorf/DE)
11:00 O–MI 06	Twin microstructure in 10M Ni-Mn-Ga martensite Werner Skrotzki (Dresden/DE)
11:20 O–TA 25	Laser-based additive manufacturing – a new processing concept for titanium aluminides Ariane Straubel (Dresden/DE)
11:40 O–TA 26	Creep properties of Ti-48Al-2Cr-2Nb produced by selective electron beam melting Vera Juechter (Erlangen/DE)
12:00 O–TA 27	Phase distribution in a lamellar Ti-42Al-8.5Nb alloy produced by powder metallurgy Heike Gabrisch (Geesthacht/DE)
12:20–14:00	*Lunch*

P–01 The influence of barrier layers (SiO_2, Al_2O_3, W) on the phase formation of RuAl thin films on LGS and CTGS substrates for surface acoustic wave technology
Marietta Seifert (Dresden/DE)

P–02 A new method to study the composition dependence of mechanical properties of Laves phases
Wei Luo (Düsseldorf/DE)

P–03 Phase transformation of thermal co-evaporated TiAl thin films on LGS and CTGS
Eric Lattner (Dresden/DE)

P–04 Compression of micropillars of single crystalline Mo_5SiB_2
Takuto Maruyama (Kyoto/JP)

P–05 Atomic scale analyses of deformation modes in Mg-TM-RE LPSO phases by STEM
Shogo Momono (Kyoto/JP)

P–06 Phase field simulation of Al_2Mg_3 and $Al_{12}Mg_{17}$ intermetallic compound formation in FSpW of AA5754 alloy to AZ31 alloy
Kuijing Song (Geesthacht/DE)

P–07 Room temperature deformation behavior of hard intermetallics and ceramics investigated by micropillar compression tests
Yasuharu Shinkai (Kyoto/JP)

P–08 Micropillar compression of single crystals of $L1_2$-Co_3(Al,W)
Zhenghao Chin (Kyoto/JP)

P–09 Precipitation behavior of Co_7Nb_2 from supersaturated Co solid solution in the Co-Nb binary system
Toshiaki Horiuchi (Sapporo/JP)

P–10 Primary phase fields of complex metallic alloy phases in the Al-Mg-Zn System close to the Mg-Zn subsystem
Guido Kreiner (Dresden/DE)

P–11 Microstructural investigation of the intermetallic composites NiAl-(34-x)Cr-xMo before and after creep
Antje Krüger (Eggenstein-Leopoldshafen/DE)

P–12 The massive transformation in a quaternary Ti-Al-Nb-Ta alloy
Marcus Rackel (Geesthacht/DE)

P–13 Determination of the crictical resolved shear stress in a NiAl-Cr composite by discrete dislocation dynamics
Gakam Herve (Karlsruhe/DE)

P–14 Atom probe study of ω_o-phase in a β-phase containing TiAl alloy
Thomas Klein (Leoben/AT)

P–15 Microstructure and phase constitution of intermetallic layers fabricated by selective laser melting of elemental Al and Ti powders
Pavel Krakhmalev (Karlstad/SE)

P–16 $Ga_{1-x}Sn_xPd_2$ ($0 \leq x \leq 1$) as catalytic material for the semi-hydrogenation of acetylene
Oksana Matselko (Dresden, Lviv/DE, UKR)

P–17 The C15 Laves phase in system U-Zr-Mo
Nathanael Wagner Morais (São Paulo, Ipero-SP/BR)

P–18 The effects of annealing on the microstructure and mechanical properties of f.c.c./B2 $Fe_{28}Ni_{18}Mn_{33}Al_{21}$
Bin Hu (Hanover/US)

P–19 Laser cladability of gradient multi-layers in Fe-Al intermetallic system
Igor Shishkovsky (Samara, Saint Etienne/RU, FR)

P–20 Void-free interconnection through dual-phase intermetallics in solid-liquid interdiffusion bonding
Tung-Han Chuang (Taipei/TW)

P–21 Mechanical properties of a forged Fe-26Al-1.5Ta compressor blade
Saeid Lotfian (Düsseldorf/DE)

P–22 Fundamental studies on casting of iron aluminides
Bruna Niccoli Ramirez (São Paulo/BR)

P–23 Solidification processing of Nb silicide based alloys – alloy design and macrosegregation of alloying additions
Panagiotis Tsakiropoulos (Sheffield/UK)

P–24 Combined *ab initio*, semiempirical and experimental approach
Jana Pavlů (Brno/CZ)

P–25 *Ab initio* and phase-field study of the Ti-Fe eutectic system
Martin Friák (Düsseldorf/DE)

P–26 Experimental investigation and thermodynamic modeling of Al-Mo-Ni System and its extension into NiAl-Cr-Mo system
Jian Peng (Karlsruhe/DE)

P–27 Integration of thermodynamic energies in phase-field simulations: ternary solidification
Michael Kellner (Karlsruhe/DE)

P–28 Crystal structures of three Ni-Ti-Si containing silicides and their oxidation resistance in air
Florian Brix (Vandoeuvre lès Nancy/FR)

P–29 Phase Stability of FeCr-σ Phase in Fe-Cr-Ni-M Quaternary System at Elevated Temperatures
Yoshiki Kumagai (Tokyo/JP)

P–30 High pressure synthesis and thermoelectric properties of phases in the Eu-Al-Si system
Alexandra Zevalkink (Dresden/DE)

P–31 Phase Equilibria among β/α2/γPhases in γ-TiAl Alloys with Combined Addition of β-stabilizing Elements at 1073 K
Hirotoyo Nakashima (Tokyo/JP)

Karlsruher Institut für Technologie

ABSTRACTS

Intermetallics 2015

28 September – 02 October 2015

O–IT 01

Novel Design Principles using TCP Phases in Austenitic Heat Resistant Materials
Masao Takeyama[1]

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Topologically close-packed (TCP) phases consisting of transition metal (M) elements, such as Laves (*C*14, hP12) and Sigma ($D8_b$, *tP*30) phases, are commonly observed but exclusively avoided for high-temperature alloy design, because of their brittle nature associated with their complicated crystal structures. Is this concept true? If yes, how about transition metal carbides, such as $M_{23}C_6$ ($D8_4$, cF116) and MC (*B*1, *c*F8)? Do they deform? These carbides are even harder than TCP phases and commonly used as strengthening species in heat resistant steels and alloys. In contract, there are no commercial austenitic heat resistant steels strengthened by TCP intermetallic phases. Why? This is because TCP phase are implicitly believed to deteriorate the mechanical properties. This thought is not necessarily true, and TCP phases can be rather promising strengthening species if their precipitation morphology can be controlled. In this talk, a novel design concept for development of a new class of austenitic steels strengthened by Laves phase is presented, based on thermodynamics and precipitation kinetics at elevated temperatures. The carbon free model steels exhibits excellent creep properties at 1073 K, equivalent to Ni-based alloys. This superior creep strength is caused by precipitation of Fe_2Nb Laves phase at the grain boundaries. The higher the fraction of grain-boundaries covered by the Laves phase (ρ), the lower the creep rate (ε), with following relationship: $\varepsilon = \varepsilon 0(1-\rho)$, leading to longer rupture life. This strengthening method, named "*Grain-boundary precipitation strengthening*", is effective at ρ>80% under low stress levels. The details of the morphology control of the Laves phase as well as the strengthening mechanism will also be presented. The design principle can be applicable to sigma phase, and some of the examples will also be touched.
Part of this study was carried under the research activities of "Advanced Low Carbon Technology Research and Development Program" (ALCA) in JST (Japan Science and Technology Agency).

O–IT 02

TiAl alloy technology trends and future opportunities in aircraft engines
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[2]GE Aviation, Cincinnati, United States

The present presentation will describe the development of TiAl alloys for commercial aircraft engine applications. The GENX™ engine is the first commercial aircraft engine that is using titanium aluminide (alloy 4822) in the Boeing 787 and 747-8. The use of TiAl in GE engines was announced in 2006. More recently, the use of TiAl in engines for the Airbus 320 and the Boeing 737 has been announced. The GENX™ engine provides a major advance in propulsion efficiency, a reduction in fuel consumption, and a reduction in noise and NOx compared to prior engines, such as the General Electric CF6.

This presentation will describe the technical principles of TiAl 4822, and the history of implementation of TiAl in low pressure turbine blades. GE has developed a range of manufacturing approaches for TiAl blades, including overstock conventional gravity casting and near net shape casting approaches. To date more than 80,000 TiAl low pressure turbine blades have been manufactured for the GENX™ 1B (Boeing 787 series) and GENX™ 2B (Boeing 747-8) applications. Production has also started on smaller thrust engines, such as the Pratt and Whitney PurePower™ 1000G engine, and the CFM LeapX™ engine. These use of second and third generation TiAl alloys will be discussed. Potential future applications will also be described.

O–IT 03

Fatigue strength in γ-TiAl produced by additive manufacturing – a few lessons learnt

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As the aeroengine industry (and the transport industry at large) is constantly increasing its interest in exploiting the advantages offered by the development of intermetallic alloys based on γ titanium aluminides, enhanced materials properties satisfying more demanding design requirements are needed, so that novel designs with high levels of structural integrity can actually be brought to the market. In the last few years, huge efforts have been made to explore new manufacturing technologies, with distinctive levels of sophistication and complexity, able to overcome the difficulties and the limitations of conventional technologies in producing γ-TiAl materials with the required properties and low defects content. Among them, additive manufacturing based on (selective) Electron Beam Melting (EBM) can be used to effectively produce γ-TiAl alloys with the specified microstructures. However, further efforts are needed to identify the relevant mechanical behaviour of these alloys in view of application to structural components.

In this work, a review of the fatigue properties of three different variants of γ-TiAl intermetallics is presented: results of fatigue tests on a Ti-48Al-2Cr-2Nb alloy, on a high Nb containing and a Mo-containing alloys, all produced by additive manufacturing by selective Electron Beam Melting (EBM) are compared, with the aim of highlighting, when possible, the effect of the microstructure on the fatigue properties. In particular, crack growth experiments conducted in the threshold region reveal how the local microstructure influences local damage accumulation processes. Additionally, specific monotonic and cyclic loading experiments with sub-size samples have been conducted for investigating the influence of the microstructure in the strain accumulation process by fatigue loading through the use of high-resolution Digital Image Correlation (DIC). The DIC analysis provides insightful information on the role of the intermetallic phases on the fatigue behaviour of γ-TiAl alloys and, by allowing a comparison between different heat treatments and resulting lamellar colonies size, permits to highlight the influence of the position of grain boundaries and the orientation of the lamellae for the onset of fatigue cracking. The analysis and comparisons of different microstructures and alloy formulations presented here is aimed at providing information for the selection of the microstructures suitable for designing against fatigue with γ-TiAl intermetallics.

Acknowledgements
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O–IT 04

***Ab-initio* based assessment of the thermodynamic stability of Al-based intermetallic phases**

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Despite the long-standing consideration of Al-based alloys such as Al-Mg-Si-Cu as light-weight structural materials, the assessment of their phase diagrams has not yet been completed. The thermodynamics and calorimetry of intermetallic phases are key ingredients in this process. We have used a set comprehensive *ab initio* methods, in order to determine the temperature depend Gibbs energies of relevant intermallic phases, ranging from binaries such as Mg_2Si [1] up to the quaternary Q phase [2]. The resulting heat capacities have been compared with recent experiments and have been used for the improvement of Calphad databases.

Within this presentation, some of the corner stones for the underlying *ab initio* thermodynamics will be presented focussing on the impact of anharmonicity and soft-phonon analysis. We will demonstrate how the calculation of the former can be significantly accelerated by the use of asymmetric nearest-neighbour potentials [3] and how the latter decisively improves the consideration of sublattice-mixing. In this context the applicability of classical concepts such as Grüneisen theory, Kopp-Neumann rule and compound-energy formalism will be critically evaluated, yielding new insights for the performance of Al-based alloys.

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[2] J. Gröbner, M. Hampl, R. Schmid-Fetzer, A. Löffler, H. Engelhardt, M. Rettenmayr, A. Zendegani, F. Körmann, T. Hickel, J. Neugebauer, Quaternary Al-Mg-Cu-Si Q-phase: Sample preparation, heat capacity measurement and first principles calculation, in preparation
[3] A. Glensk, B. Grabowski, T. Hickel, and J. Neugebauer, Understanding anharmonicity in fcc materials: From its origin to *ab initio* strategies beyond the quasiharmonic approximation, Phys. Rev. Lett. (accepted)

O–IT 05

Effective cluster interactions and intermetallics thermodynamics
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The most successful statistical thermodynamics models in material science rely on decomposing the internal energy of the system into effective cluster interactions (ECIs), attributable to groups of interacting atoms (the "clusters", like pairs, triangles, tetrahedra and so on). This allows the application of several approaches to solve the complex statistical mechanical problem of calculating the alloy entropy, hence obtaining the system's Gibbs free energy. As a result, ordered intermetallics appear as a "natural" solution of these models, when interactions of unlike atoms become predominant. This decomposition of the internal energy into "cluster interactions" is so successful, that it is often used in introductory materials thermodynamics classes around the world as an example of "materials" application. The physical nature of the ECIs, however, has been a subject of controversy in the specialized literature and, more recently, the advent of modern quantum mechanical models for the calculation of electronic structure allowed the direct determination of these parameters, with the obvious results that they can be checked against experimental data on compound thermodynamics and phase equilibria. The aim of the present work is to review and clarify the context in which ECIs are introduced in the different formalisms introduced in the XXthcentury, in particular the early attempts of using the Ising model to calculate phase diagrams of ordered alloys, the formalism of Bieber and Gautier, with their "concentration dependent" ECIs, the cluster expansion method (CEM) and modern *ab initio* phase diagram calculation, and the position dependent cluster interactions in the context of the Continuous Displacement–Cluster Variation Method (CD-CVM). The perspectives for the future in the field will be discussed.

O–IT 06

Phase stability and mechanical properties of high-entropy alloys
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Our physical metallurgy intuition tells us that the greater the number of elements in metallic alloys the higher the probability of intermetallic phase formation by reaction among the constituents. As a counterpoint, it has been hypothesized that formation of intermetallics can be suppressed if the configurational entropy of competing solid solution states is sufficiently high. This has generated significant interest in the new class of so-called high-entropy alloys containing five or more elements in equiatomic proportions. Here we examine the role of configurational entropy in suppressing intermetallic phase formation by analyzing the microstructures of various alloys in the cast and homogenized state, as well as after various thermomechanical treatments. The mechanical properties of the alloys are then discussed and correlated with the evolution of microstructure, including the embrittlement caused by intermetallic phase formation in an otherwise ductile FCC high-entropy alloy.

O–IT 07

Combinatorial materials research for novel intermetallic alloy systems

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The directed and efficient discovery and optimization of materials is a key challenge in materials science. New materials for actuation in MEMS as well as new materials for the sustainable production/storage/conversion of energy carriers are necessary to improve existing and enable future products. By implementing and optimizing the combinatorial materials science approach in our group during the last ten years, we are trying to contribute to this development. It comprises the fabrication and processing of thin film materials libraries by several combinatorial sputter deposition processes (40 elements available) and optional post-deposition treatments (e.g. annealing, thermal oxidation), followed by the high-throughput characterization of the different thin film samples contained in these libraries, and in a last step the up-scaling of findings from materials libraries to larger sizes. Our high-throughput material characterization methods are automated, fast, and mostly non-destructive: examples are EDX and RBS for composition, XRD for crystal structure, temperature-dependent resistance for phase transformation, high-throughput test stands for optical properties and mechanical properties (stress, hardness, elastic modulus). The obtained results for ternary and quaternary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover combinatorial exploration of intermetallic systems with regard to identifying unknown phases as well as to explore the compositional ranges of the observed phases. Examples of the combinatorial exploration of intermetallic material systems for shape memory (Ti-Ni-X-Y, Ti-Ta-X) and thermoelectric (Ti-Ni-Sn) applications as well as results on the investigation of ternary subsystems of Ni- and Co-based superalloys (Ni-Al-X, Co-Al-X, Co-Ni-Al, Co-Ti-W, …) will be discussed.

Funding of the DFG (SFB TR103, Forschergruppe 1766, …) is acknowledged, as well as the work of the team members and cooperation partners in these projects.

O–IT 08

High temperature Mo-Si-B alloys – phase stability and environmental resistance

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The challenges of a high temperature environment (T>1400°C) impose severe material performance constraints in terms of melting point, oxidation resistance and structural functionality. In metallic systems there are several high melting temperature intermetallics, but there is a much smaller number of intermetallic phases that offer a level of inherent environmental resistance. Moreover, above about 1300°C, SiO_2 films are preferred since the parabolic rate constant is lower for SiO_2 than for Al_2O_3. However, single phase silicides such as $MoSi_2$ are brittle so that multiphase designs are necessary. The multiphase microstructures that can be developed in the Mo-Si-B system offer useful options for high temperature applications. Alloys based upon the coexistence of the high melting temperature (>2100°C) ternary intermetallic Mo_5SiB_2 (T_2) phase with Mo and the Mo_3Si phase allow for *in-situ* toughening and offer some oxidation resistance. A focal point of the microstructural designs is the T_2 phase which exhibits a range of solubility. Selected refractory metal substitutional alloying has been examined to alter the solubility of the T_2 phase and the relative phase stability as a method to develop multiphase microstructure design options. The observed alloying trends also highlight the fundamental geometric and electronic factors that influence the relative stability of the T_2 phase. Similarly, the systematic investigation of reaction kinetics involving the T_2 phase has a direct application to the analysis of oxidation behavior and to the design of effective coating systems based upon a kinetic bias strategy. In order to achieve a compatible interface coating together with enhanced oxidation resistance, a pack cementation process has been adapted to apply diffusion coatings. From this basis protective coatings are being developed with an *in-situ* diffusion barrier, self-healing and gradient characteristics. The environmental resistance can be enhanced up to at least 1700°C and also extended against attack by water vapor and CMAS. With these advances the multiphase microstructures that can be developed in Mo-Si-B alloys offer useful options for ultrahigh temperature applications.

O–IT 09

Application of chevron-notched micro-size fracture testing method on single crystal Si and Nb-Si intermetallic compound

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A micro-sized fracture testing on small cantilever specimens with a chevron-notch is conducted on Si single crystal and Nb-Si intermetallic compound. Specimens with a size of approximatery 3 ×3 × 15 μm^3 were prepared using a focused in beam, FIB, technique at the edge of bulk materials. Fracture tests were conducted using a nanoindenter at room temperature and the fracture behavior was compared with bulk samples. The evaluated fracture toughness K_Q are in good agreement with the value of bulk samples. Also the Nb/Nb_5Si_3 inter-phase boundary cracking behavior was investigated.

O–IT 10

Effects of vacancy-site occupation on phase stability, thermoelectric properties, and mechanical behavior of half-Heusler MNiSn (M: Ti, Zr, Hf) alloys

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Thermoelectric power generation is an appealing approach for the energy conservation and environment preservation. We are focusing on half-Heusler type MNiSn (M: Ti, Zr, Hf) phase as excellent n-type thermoelectric materials for high temperature applications. Thermoelectric properties as well as mechanical properties of half-Heusler compounds can be improved, or affected, by the distinctive microstructure, lattice defects, and interfaces, which are formed due to the crystallographically and thermodynamically close relationship with Heusler MNi_2Sn compounds, since their ordered structures resemble each other. Objective of the present work is to understand how these types of distinctive microstructure are formed based on phase equilibria, and to evaluate their effects on the thermoelectric properties, and mechanical behavior as well. Microstructure observation and crystallographic analyses were conducted using the scanning-transmission electron microscopy (STEM) and the X-ray diffractometry. Thermoelectric properties were evaluated by measurements of Seebeck coefficient, electrical resistivity and thermal conductivity. Several hundred micrometers size single crystals of stoichiometric TiNiSn were grown using the solid-TiNi and liquid-Sn reaction at the interface, and those of slightly Ni-rich TiNiSn were fabricated by the unidirectional solidification using optical floating zone melting. Nano-sized Ni-rich clusters, which we denoted as a modulated-like nanostructure, is observed using STEM in Ni-rich TiNiSn phase as blocky domains, which function as precursor for Heusler nano-precipitates. A similar modulated-like nanostructure is observed even in the stoichiometric TiNiSn phase as point defects which are supposed to form in a process that Ni atoms and vacancies randomly swap their positions in the Ni-Vacancy sublattice. The vacancy-site occupation was investigated in the $M(Ni,Co_x)_{1+x}Sn$ (x = 0~1) quaternary systems. The n-type thermoelectric properties of TiNiSn can be converted to the p-type by the vacancy-site occupation with Co, as same as we previously reported for ZrNiSn. The solubility of Co in the vacancy-site of TiNiSn is much larger, while its effect on the Seebeck coefficient conversion is smaller than those in ZrNiSn. On the other hand, the solubility of Co in HfNiSn is limited very small.

Compression tests were conducted at elevated temperatures on several half-Heusler (HH) with or without vacancy-site atoms and Heusler (H) alloys. All the alloys fracture within elastic region before the yielding at 1173 K, however, they exhibit plastic deformability at 1273 K in compression. The yield strength, evaluated as the 0.2% proof stress, at 1273 K is about 250 MPa for HH-ZrNiSn and about 100 MPa for H-$ZrNi_2Sn$. The yield strength at 1273 K is higher in the order of HH-ZrNiSn, HH-$Zr(Ni,Co_{0.25})_{1.25}Sn$, HH-$Zr(Ni,Co_{0.75})_{1.75}Sn$, H-$Zr(Ni,Co)_2Sn$, H-$ZrNi_2Sn$.

O–IT 11

Synergies between theoretical and experimental methods in modern materials science: an insight from *ab initio* calculations

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State-of-the-art quantum-mechanical (so-called *ab initio*) methods constitute a solid basis of modern theoretical materials science and computational materials design. *Ab initio* calculations represent a unique source of information whenever experimental data are missing and provide also a deeper insight and fundamental understanding. The talk will exemplify synergies between quantum-mechanical calculations and advanced measurements in case of multi-component materials intended for cutting-edge industrial applications. The first example will be high-strength dual-phase Fe-Ti eutectics containing FeTi intermetallics. Studying a broad range of Ti concentrations we have identified fundamental relations connecting electronic-structure properties of constituting phases with their thermodynamic stability and macroscopic elastic characteristics. Second, an impact of local stresses on the microstructural stability at elevated temperatures will be shown in case of Laves phases stabilizing novel ferritic steels. Third, focusing on nano-patterned CrN/AlN high-performance superlattices, epitaxial stresses will be presented as a newly emerging groundbreaking materials-design concept providing exotic phases that would otherwise not exist in strain-free bulk systems. Next, the thermodynamic stability of a five-component magnetic high-entropy alloy will be examined with respect to decomposition into less-component intermetallic phases. Lastly, as internal interfaces are essential for a reliable description of any realistic material, solute-mediated grain boundary engineering will be exemplified in case of selected clean and impurity-decorated grain boundaries in Ni_3Al.

O–IT 12

Nickel-titanium-hafnium alloys with high strength and advanced functional performances

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In recent efforts, we have successfully identified new alloy compositions and processing techniques that mitigate functional fatigue cycling behaviors of both actuation and superelastic responses of shape memory alloys. Specifically, by substituting small to modest amounts of hafnium for titanium, a new intermetallic phase may form that is compatible with the shape-memory behavior enabling crystal structures. Furthermore, the phase may provide tremendous structural strength (2 to 3 GPa) and eliminate hysteresis from functional responses. We will present fundamental *in-situ* diffraction studies of the deformation mechanisms and microstructures of these new advanced alloys. We will also discuss the development of two specific compositions of these alloys for applications that include aerospace actuation as well as use in corrosive or shock-prone tribology environments.

O–IT 13

Mechanical properties of novel polycrystalline Co-base superalloys with $L1_2$ ordered precipitates

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[1]University of Erlangen-Nürnberg, Materials Science & Engineering, Erlangen, Germany

Intermetallic phases are essential for strengthening of alloys that are used for high temperature applications. Ni-base superalloys, for example, exhibit excellent mechanical properties due to a high volume fraction of ordered Ni_3Al precipitates with $L1_2$ crystal structure that are coherently embedded in a fcc solid solution. In 2006 another type of this group of $L1_2$ phases, $Co_3(Al,W)$, was discovered that has led to the development of novel Co-base superalloys with attractive properties. They have very high solidus temperatures and although the solvus temperature of the intermetallic compound is comparatively low, high volume fractions of the $L1_2$ phase at temperatures up to 900°C can be achieved. Thus, high-strength polycrystalline Co-base superalloys with intermetallic precipitates can be produced by the conventional cast-and-wrought method. In this work the development and properties of this new class of high temperature materials will be presented and discussed. The solidus temperatures of our multinary Co-base superalloys are above 1300°C and the solvus temperatures between 1000°C and 1100°C. The fraction of the $L1_2$ phase is above 50% and high energy X-ray diffraction measurements show that the lattice parameter of the $L1_2$ phase is in general larger than that of the unordered fcc matrix phase. The oxidation resistance is much better compared to that of ternary Co-Al-W based superalloys. In comparison to conventional Ni-base superalloys compression tests show that a higher yield strength above 800°C could be achieved and the creep strength is superior at 750°C.

O–TA 01

Formation of a fine and resistant microstructure in TiAl alloys by spark plasma sintering
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[1]CEMES/NRS, Toulouse, France

During the last decade, TiAl alloys have been successfully produced by Spark Plasma Sintering (SPS). SPS is a powder metallurgy technique, for which the heating of the sample occurs by the application of a pulsed direct electric courant. This process allows achieving original microstructures with enhanced properties due to its rapid processing cycle as well as non-textured, homogeneous structures as with all powder metallurgy techniques.

To obtain alloys with high mechanical properties with this process, our choice was to look for a fine, homogeneous microstructure. The aim of the present talk is to describe the route to obtain such a microstructure which is made of small lamellar grains surrounded by singe-phased γ borders. In particular, we will focus on the influence of the chemical composition and of the SPS cycle. The microstructures are studied by scanning and transmission electron microscopies. A formation mechanism of this microstructure will be proposed in consistency with our experimental results and with experimental and calculated phase diagrams.

O–TA 02

TiAl revert conversion into feed stocks for the production of aircraft engine components
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Different manufacturing technologies have been established for the production of TiAl low pressure turbine blades, whereas the production of appropriate pre-materials (feed stocks) is mainly based on VAR skull melting and subsequent centrifugal casting in permanent moulds. During this process a remarkable part of the liquid TiAl solidifies in feeders, on the casting plate or in the tundish system as valuable bulky revert. Furthermore, such revert results from subsequent processing steps (gatings and risers from investment casting, forging edges, cut-offs etc.) as well. With rapidly increasing production volumes, the recycling of revert is mandatory to meet cost reduction requirements. The most common recycling technology in the Titanium industry is the scrap conversion into ingots via PAM or EBM which allows to produce any kind of Ti products such as bars, profiles, sheets, tubes, foils and others. With regard to TiAl, the number of different semi-finished products is very limited. Moreover, sizes and shapes of the different feed stock are more or less similar to each other. This offers the opportunity to commercialize a one step recycling technology direct into semi-finished products. GfE has developed the revert conversion via VIM skull melting and subsequent centrifugal casting into permanent moulds. A VIM SM furnace has been commissioned recently. First results are being reported which give evidence that the resulting products from VAR skull melting and VIM skull melting both with subsequent centrifugal casting into permanent moulds exhibit comparable technical properties.

O–TA 03

Manufacturing and properties of TiAl TNM® sheet materials
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It has been demonstrated that β-solidifying TiAl alloys such as the TNM® alloy exhibit a remarkably improved wrought processing capability in comparison to conventional γ-based TiAl alloys. Based on TiAl TNM feed stocks manufactured via GfE VAR skull melter processing, a TiAl sheet manufacturing technology has been developed in the lab scale which offers the opportunity for an industrial commercialization. Since the centrifugally cast and HIPed feedstocks exhibit a very homogeneous and fine grained microstructure, any prior ingot conversion into powders or fine grained extruded profiles is not needed. Rolling has been performed on air using a conventional two high mill down to a thickness in the as-rolled state of 1.5 mm. The sheet dimensions of 300 mm x 500 mm x 1 mm are limited by the lab equipment but not by the technology itself. Sheet materials properties such as microstructure, tensile properties, hardness and SPF processing capability have been evaluated. The production of complex shaped parts such as aircraft engine exhaust system components could be successfully demonstrated.

O–TA 04

High-speed die forging of TiAl alloy
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Wrought TiAl alloys show good mechanical properties such as creep strength, tensile strength and fatigue strength. However wrought TiAl alloys have bad forgeability and require caning, slow forging. Therefore wrought TiAl alloy is more expensive than wrought Ni base alloy for the small parts. To reduce the cost, higher speed of die forging and caning less are essential for TiAl alloys. The aim of present work has been the development of high speed die forging technique. Hot forgeability was assessed by the compression test and the gleeble test in the range from1100 to 1350 degree C.

Test materials with different microstructure were prepared by some heat treatment. Microstructure altered the volume fraction of lamellar colony, β phase volume fraction and grain size. High temperature ductility depended strongly on prior grain size, the volume fraction of lamellar colony. In addition, high temperature ductility was significantly affected by test conditions such as the deformation rate and the atmosphere.

On the basis of these results, the die forging tests were conducted under the optimized condition. The die forging test deformed from 25 to 5mm under high speed were became successful.

O–TA 05

***In situ* synchrotron radiation study during hot forming of a Nb-rich TiAl alloy**

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An active and actual research and development topic is the development of suitable hot forming processes, e.g. forging routes, for mass production of TiAl parts. Recent research activities are focused on TiAl alloys containing additional amounts of ductile bcc high-temperature β phase due to their improved formability at elevated temperatures.

We studied the hot forming process of a Nb-rich TiAl alloy using a deformation dilatometer (DIL 805A/D) that was modified for working in the HZG synchrotron radiation beamline HEMS at DESY. This setup enables an *in situ* observation of the interaction and evolution of several microstructure parameters during hot forming. The method yields direct information about processes which are otherwise masked by post process alterations as phase transformations or recrystallization. Thereby, the evolution of phase fractions, grain size and crystallographic texture was directly observed during deformation while simultaneously recording the process parameters, temperature, force and length change.

The alloy had a nominal composition of Ti-42Al-8.5Nb (in at.%). We performed several hot compression tests at different process temperatures. Thus, the phase fractions in the alloy vary from equal fractions of γ-TiAl and α_2-Ti_3Al at 1100°C to mainly α-Ti(Al) at 1200°C, and α-Ti(Al) + β-Ti(Al) at 1300°C. Thereby, it was possible to analyse the interactions between the different phases during processing. The samples were deformed with strain rates from 2E-3/s to 3E-2/s each up to a total reduction of about 45%. Immediately after deformation most samples were quenched to retain the deformed microstructure. Additionally some samples were heat treated to study the influence of static recrystallization on the deformation texture.

This kind of *in situ* studies during deformation and subsequent annealing can provide new insights into the interaction between deformation, recrystallization and phase transformation and the formation of the final texture and allows a more detailed optimization of process parameters regarding final alloy properties.

O–TA 06

A new processing route for forged TiAl automotive engine valves

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For application as exhaust valves in automotive engines, γ-TiAl alloys offer the potential of weigh reduction and increased working temperature compared to other traditional heat-resistant materials. The key to realizing mass production is to achieve a balance between mechanical properties that meet service requirement and acceptable processing cost. In this study, a new processing route was attempted and sections of an α solidifying alloy (Ti-47Al-2Cr-2Nb-0.15B, at%) were first made into pancakes through primary canned forging. Bars extracted from the pancakes were then made into preforms of valves through secondary closed die forging at T_{α}-20˚C. Such a two-step hot-working scheme plus subsequent heat treatment in the γ phase region for a short time produced fine homogenous fully lamellar microstructure as well as desirable flowlines and texture of the preforms. The hot workability and microstructural evolution during the processing will be discussed. Exhaust valves made in this processing route were supplied to an automobile company.

O–TA 07

Microstructure and texture characteristics of extruded Ti-47Al-2Cr-2Nb-0.15B with different initial microstructure of billets

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The microstructure and texture of Ti-47Al-2Cr-2Nb-0.15B after extrusion in the α+γ phase field were studied in this work. Three types of starting microstructures were employed: equiaxed of a HIPed powder billet, duplex of a forged billet, and fully lamellar of a forged billet. While extrusion produces fully fragmented equiaxed microstructure from the first two types of billet, some lamellae remained after extrusion for the third type of billet. The largest and finest grain size of both equiaxed α_2 and equiaxed γ were obtained in billets having duplex and fully lamellar microstructure, respectively. EBSD analysis showed that after extrusion all the billets have strong α_2 phase texture {11-20}<10-10>, while {0001}<10-10> texture was found in the fully lamellar billet and near <0001> fiber texture was found in the forged billets. Cubic texture component of γ phase was found in all the samples, but its intensity, like that of other texture components of γ phase, varied with the initial billet microstructure. Texture components of α_2 and γ phase in all the samples were compared, and their evolution mechanisms were discussed.

O–TA 08

Microstructure formation and phase composition in diffusion brazed γ-TiAl-alloy joints

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Diffusion brazing is a promising method to close cracks (in noncritical or not highly loaded areas) in parts made of TiAl alloys, for example aero engine vanes. In this work the phase constituents, phase distribution, and microstructure of the joint zone of diffusion brazed Ti-45Al-5Nb-0.2B-0.2C (in at. %) alloys are investigated. Two brazing alloys based on Ti-Fe and Ti-Ni are used.

The phases and their distribution in the brazing zone were determined by high-energy X-ray diffraction (HEXRD) using the materials science beamline HEMS at the PETRA III synchrotron facility at DESY in Hamburg, Germany. In addition, *in-situ* studies of the brazing process were performed. Furthermore, the microstructure was characterised by scanning electron microscopy (SEM) including energy-dispersive X-ray spectroscopy (EDX) and electron backscattered diffraction (EBSD). The combined results show, that the brazing zone is composed of two or three transitional layers from substrate material to the middle of the joint. While the phase constitution
close to the substrate material resembles a TiAl-alloy, the microstructure in the middle of the joint is similar to α/β-titanium alloys. Tensile tests showed that a fine grained microstructure in the joint zone is in general favourable for mechanical strength. The grain size in the joint zone differs significantly between both brazing alloys. The reason for this can be understood based on the development of the phase constitution over brazing time observed in the *in-situ* HEXRD investigations.

O–TA 09

Large scale forging of an advanced Ti-Al-Nb alloy

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The advanced low aluminum, high niobium containing TiAl alloy Ti-42Al-8.5Nb (nominal composition in at.%) exhibits an excellent combination of high-temperature strength and room temperature ductility. This alloy has a nano scale modulated microstructure consisting of lamellae with a tweed substructure. These tweed-like appearing lamellae are an arrangement of multiple stable and metastable phases with at least one orthorhombic constituent. The nature of the orthorhombic phase as well as its formation path was directly observed and identified using *in situ* high-energy synchrotron X-ray diffraction (HEXRD) measurements. Based on the results the amount of O phase can be adjusted through heat treatments. Several deformation tests and HEXRD experiments were performed to develop a thermo-mechanical processing route for this Ti-Al-Nb alloy. The derived parameters were directly used to forge large scale parts under industrial conditions. Cylindrical rods of 100 mm in length and 55 mm in diameter were forged at 1235°C with nominal strain rates of 0.01 s^{-1} and 0.005 s^{-1} under nitrogen atmosphere. The as forged microstructure and the microstructure after post processing heat treatments were characterized by SEM and EBSD measurements. Additionally, tensile testing was performed to characterize the mechanical properties at room temperatures.

O–TA 10

Measuring plastic deformation of titanium aluminides under compressive and tensile uniaxial loading using sub-micron resolution digital image correlation and Kikuchi diffraction mapping

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Improving the fatigue behaviour of γ-TiAl requires an understanding of crack nucleation and how this is related to the detailed microstructure. The monotonic compressive and tensile deformation behaviour of a γ-TiAl alloy (Ti-45Al-2Nb-2Mn(at.%)-0.8vol.%TiB_2) with a range of different lamellar thicknesses has therefore been measured at both room temperature and at 700°C. Both colony and lamellar-scale deformation features of the material have been investigated. The lamellar structures were characterised by scanning electron microscopy and transmission Kikuchi diffraction. The near-surface plastic strain field and the build-up of local strains have been measured, using digital image correlation, with a remodelled gold speckle pattern, and compared with misorientation mapping using electron backscatter diffraction, both before and after testing. The lamellar thickness was found to affect the translamellar deformation produced, which in preferentially oriented colonies resembled kink bands, characteristic of lamellar composite materials. This is related to the possible accumulation of damage in cycling loading.

O–TA 11

Describing the temperature-dependent yield point of polysynthetically twinned TiAl crystals by means of a thermomechanically coupled crystal plasticity model

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The macroscopic deformation behavior of fully-lamellar TiAl alloys is influenced by numerous micromechanical mechanisms on the meso scale. A reliable prediction of the yield point, as it is needed in construction design, therefore requires a respective material model to describe the micromechanics of the lamellar compound. Polysynthetically twinned TiAl crystals are well suited to be analyzed with respect to their micromechanical behavior since they basically consist of a single lamellar colony free of the influence of neighboring colonies.
In the past, various crystal plasticity-based models were set up to describe the plastic deformation behavior of polysynthetically twinned TiAl crystals at room temperature. The plastic anisotropy as well as the Hall-Petch related strengthening were incorporated in most of the reported models in one way or another but the material behavior at elevated temperatures was never addressed. However, since the preferred operating temperature for TiAl alloys is in the range of 500°C-700°C, the influence of the temperature on the plastic deformation behavior has to be considered in a respective model. To do so, a thermomechanically coupled crystal plasticity model is set up and implemented into a commercial finite element code. The formulation of the model accounts for structural heating due to plastic deformation and considers the temperature dependence of the model parameters. Here, special emphasis is placed on the anomalous rise of yield stress with temperature, as it is observed in polysynthetically twinned crystals. This flow stress temperature anomaly as well as the influence of the various phase boundaries on the yield stress are incorporated into the model via the critical resolved shear stresses. The simulation results are in good agreement with experimental findings.

Reference:
Butzke, Bargmann, Thermomechanical modeling of polysynthetically twinned TiAl crystals, submitted, 2015

O–TA 12

Segregation of C and Si in lamellar microstructures of β-solidifying γ-TiAl-based alloys

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Intermetallic γ-TiAl-based alloys, as light-weight high-temperature materials, merit significant attention due to their potential to substantially reduce fuel consumption and environmental impact of aero and automotive engines. Facilitating aspects pertaining to their applicability are a low density, a high creep resistance as well as a high strength and modulus retention at elevated temperatures. The highest creep resistance can be achieved by so-called fully lamellar microstructures and, moreover, can be positively influenced by alloying with C and Si.

Aim of this study was the investigation of the microstructural evolution of the so-called TNM$^+$ (Ti-43Al-4Nb-1Mo-0.1B-0.3C-0.3Si) alloy, containing C and Si, by scanning electron microscopy, transmission electron microscopy and atom probe tomography (APT) during a common two-step heat-treatment, which is applied to achieve a lamellar structure. APT was employed to investigate the redistribution of alloying elements. Especially, the Si distribution in all constituent phases in equilibrium and disequilibrium states was determined. During the course of lamellar γ-phase precipitation, partitioning and segregational effects of alloying elements at interfaces were observed. These were addressed by calculation of interfacial excesses [1]. At several stages during the γ-phase formation the heat-treatment was interrupted to study the kinetics of elemental redistribution and coarsening effects.

Data gained in this study significantly contributes to the understanding of the microstructural evolution of multi-phase γ-TiAl-based alloys during application-oriented heat-treatments. Special emphasis is laid on the analysis of interfaces. Most importantly the critical role played by the alloying element Si pertaining to the microstructural evolution, preferential location and segregational effects are addressed.

[1] O.C. Hellman, D.N. Seidman, *Mater. Sci. Eng. A 2002*, *327*, 24.

O–TA 13

Carbides in γ-TiAl alloys with varying alloying elements and thermal history

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The creep resistance of γ-TiAl alloys can be improved by the addition of carbon via precipitation hardening. Two carbide types are reported in g-TiAl based alloys: perovskite (P-Ti_3AlC) type carbide and hexagonal (H-Ti_2AlC) type carbide. According to the Ti-Al-C ternary phase diagram, in γ-TiAl alloys P-type carbides are only meta-stable, while H-type carbides are thermodynamically stable. So eventually with increasing aging time or aging temperature P-type carbides should disappear and H-type carbides should form instead.

Up-coming alloys with low aluminum contents and high levels of niobium and other b stabilizing elements could be fundamentally different with respect to carbide precipitation. For example, niobium slows down diffusion, leads to a refinement of the microstructure and is reported to increase the

solubility for carbon in γ-TiAl alloys. Other aspects can also influence the formation, shape and size of carbides such as carbon concentration and thermal history.

Thus in this study the alloys Ti-45Al-5Nb-xC (x=0.5, 0.75 and 1.0), Ti-45Al-0.5C, and Ti-51Al-5Nb-xC (x=0.01, 0.05 and 0.5) (all in atomic percent) were investigated in order to understand the influence of Nb additions, Al content and thermal history on carbide formation. After different heat treatments, the carbide microstructures are characterized by high energy X-ray diffraction and transmission electron microscope.

The results show no strong influence of Nb on carbon solubility. In both Ti-45Al-5Nb-0.5C and Ti-45Al-0.5C alloys, P-type carbides are stable after over 1000 h of ageing at 800°C. With increasing Al or C concentration, H-type carbides form and exist together with P-type carbides.
The long term stability of carbides in these alloys will be discussed in the paper.

O–TA 14

Influence of niobium, tantalum and zirconium on lattice parameter and hardness of the α_2- and γ-phase in fully lamellar titanium aluminides

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Titanium aluminides represent an interesting alternative to the established nickel-based superalloys for high-temperature applications due to their high specific strength. Especially fully lamellar titanium aluminides, consisting of the two Intermetallic phases γ-TiAl and α_2-Ti_3Al, exhibit excellent creep properties.

For a more precise understanding of the influence of the alloying elements Niobium, Tantalum and Zirconium on the mechanical properties, the three model alloys Ti-44Al-5Nb, Ti-44Al-5Ta and Ti-44Al-5Zr were characterized.

The addition of alloying elements to improve the mechanical properties can have a number of effects. Third elements can for example cause a solid solution hardening and change the lattice parameter of the intermetallic phases. This was investigated with nanoindentation measurements in an atomic force microscope and high energy x-ray diffraction analysis via synchrotron radiation. The change in the lattice parameter causes a modification of the α_2/γ lattice misfit as well as a change in the a/c -ratio of the individual phases.

O–TA 15

The influence of aerofoil structure on metallurgical quality of cast TiAl turbine blades
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Centrifugal casting of net shape turbine blades of γ-TiAl alloys offers one of the low cost manufacturing routes, but it is not known how the aerofoil structure and profile correlate with metallurgical quality of the blades, an issue directly related to the yield and thus cost of production. At the moment computer simulation is not advanced enough to predict occurrence and distribution of casting defects in a centrifugal casting environment, and reliable data must be gathered from experiment. In this study 9 simulation models with different aerofoil size and shape have been orthogonally designed, and centrifugally cast under identical experimental settings. Three key aspects of metallurgical quality, forming ability, surface porosity and internal shrinkage, were quantitatively evaluated, and the data were analyzed against the aerofoil structure parameters such as maximum thickness, curvature radius and profile variation. The results suggest that the forming ability depends on the slope of the maximum thickness along aerofoil span, while the surface porosity and the internal shrinkage are mostly affected by the curvature of cross-section. Two out of the 9 models clearly have better 'castability' than others.

O–TA 16

Columnar-to-equiaxed transition and peritectic solidification in γ TiAl alloys
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Intermetallic TiAl alloys have recently found an application in the low-pressure turbine blades of aircraft engines. The Ti-48Al-2Cr-2Nb "GE" alloy combines an attractive specific strength and specific modulus with over 20 years of development and testing by General Electric. Casting is important in TiAl turbine blade manufacturing, but this processing technique can limit product quality due to structural heterogeneities and chemical segregation related to casting and solidification. The columnar-to-equiaxed transition (CET), one of the most important structural heterogeneities related to casting, leads to heterogeneous mechanical properties in cast parts. Moreover, within the composition range of interest, peritectic solidification further complicates the CET. In this experimental study, small 20-g ingots of peritectic or near-peritectic γ TiAl alloy compositions were produced via cold crucible semi-levitation and gravity casting experiments. The aluminum content of a GE-type alloy was varied to explore this range of compositions. The dimensions and grain density of the equiaxed zone of these ingots were measured using electron microscopy techniques and compared to the classical Hunt model. Microstructural observations also investigated the effects of the primary solidification phase and peritectic solidification on the CET.

O–TA 17

Influence of borides on the phase transformation kinetics in γ titanium aluminide alloys
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Due to the inherent brittleness of γ titanium aluminide alloys part of the alloy and processing development aims at fine and homogeneous microstructures. Pronounced microstructural refinement can be achieved by the addition of B, as it is known since about two decades. Recently it has been shown that this effect can be attributed to heterogeneous nucleation of the α phase on borides during the β→α transformation, which however is only observed for slow cooling rates. In order to understand the microstructural refinement the phase transformations kinetics was analyzed by *in situ* high-energy XRD on cooling the material from the high-temperature β phase field. In the experiments an inductively heated dilatometer was used for heating and cooling specimens of the alloys Ti-43Al-5Nb and Ti-43Al-5Nb-0.2B (at.%). The specimens were heated to a temperature above 1430°C, held for 1 min and then cooled to room temperature with several cooling rates from 1 K/s up to 30 K/s. The phase fractions were determined by HEXRD and in addition from the length signal measured by the dilatometer. The obtained transformation curves were quite similar except some characteristic differences. From the evolution of the transformed volume fraction the start temperature of the β→α transformation was determined for different cooling rates. For all cooling rates the transformation starts at higher temperature in the B containing alloy. Further, the experiments indicate a change in the transformation mechanism between 5 K/s and 10 K/s the origin of which will be discussed in the contribution.

O–TA 18

Centrifugal investment casting of γ TiAl automotive engine pistons
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In this work automotive engine pistons were made by centrifugal investment casting Ti-45Al-2Mn-2Nb-0.8vol.%TiB_2 alloy into shell moulds with yttria face coat. To reduce weight the piston features complex hollow structures around the pin hole, creating large stress between the top and the pin hole regions during cooling after casting. It was found necessary to reduce the local strength of the shell mould to accommodate the stress concentration and to avoid cracking of the casting. The pattern configuration was optimized to significantly reduce casting defects such as porosity and gas pores. Surface quality of the castings was evaluated using cross-sectional metallography and hardness test. Grain sizes of sections of different thickness were characterrized. X-ray inspection shows good metallurgical quality of the pistons after HIPping which meet the requirement of application.

O–TA 19

***In-situ* study of the time-temperature-transformation behaviour of an intermetallic γ-TiAl based alloy**

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TNM alloys with a nominal composition of Ti-43.5Al-4Nb-1Mo-0.1B (in at.%) belong, as intermetallic γ-TiAl based alloys, to a class of innovative high-temperature lightweight materials. In particular, they are characterised by their excellent processing characteristics, which are due to a high amount of disordered β-phase present at hot working temperatures. In a post-forging multi-step heat treatment, balanced mechanical properties can be tailored by adjusting the material's microstructure. For the optimisation of heat treatment steps, and, thus, the material's mechanical properties, information on its time-temperature-transformation behaviour is essential. In the present work, *in-situ* high-energy X-ray diffraction experiments were conducted to study a TNM alloy with an increased content of β-stabilising alloying elements Nb and Mo in a dynamic and technologically relevant context. In a dilatometer setup placed in the synchrotron radiation beam, forged and homogenised specimens were annealed in the (α+β+γ)-phase field region and subsequently subjected to cooling rates ranging from 35 to 1200 K min^{-1}. The correlation between these cooling rates and the resulting microstructures, which were analysed by means of scanning electron microscopy, was investigated with respect to the evolution of phase fractions as functions of time and temperature. The focus was laid on the evolution of the γ-TiAl phase, for which a continuous cooling transformation diagram was derived. Additional *in-situ* heating experiments close to thermodynamic equilibrium conditions, combined with quantitative metallography on heat-treated and water-quenched specimens, provided information for temperature calibration. The performed *in-situ* diffraction experiments using synchrotron radiation offered a deeper insight into the phase transformation behaviour of the investigated type of multi-phase alloy, which is not accessible with conventional characterisation techniques.

O–TA 20

Atomic relaxation processes at high temperature in Mo-rich β/γ-Ti-Al intermetallics

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Advanced γ-TiAl intermetallic alloys are being used as structural high-temperature materials, (for applications in automotive and aircraft engine industry), because of their low density and high specific mechanical properties. Due to the last decades of intensive research and development they are becoming competitive materials, but still alloy improvements are required to increase particular properties. Looking in this direction, the study of atomic relaxation processes through mechanical spectroscopy offers a fundamental tool to understand the mechanisms controlling the evolution of the microstructure at high temperature. In the present work a short overview of the internal friction and dynamic modulus measurements carried out in TNM γ-TiAl alloys will be initially presented, paying special attention to the atomic relaxation processes observed in these alloys. Then the evolution of the internal friction spectra with microstructure in Mo-rich model alloys Ti-Al-Mo with different amount of Mo has been studied. In order to lead to a better understanding of the defect mobility processes taking place at high temperature, internal friction (IF) and dynamic modulus measurements (DM) have been carried out by mechanical spectroscopy. The obtained results show two relaxation peaks, whose activation enthalpies have been determined and discussed in terms of the atomic defects mobility mechanisms. The high-temperature background (HTB) has been

also analysed in relationship with the creep behaviour. A clear correlation between the HTB, measured by mechanical spectroscopy, and the creep behaviour has been established. This correlation is discussed on the light of the recent results giving evidences of its interest for industrial applications.

O–TA 21

Stability issues at the boundary between ***in-situ*** grown oxides on selective halogenated intermetallic **titanium aluminides**

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Increasing demands on technical components for high-temperature applications (e.g. turbine blades) promote new developments not only in the field of alloy design, but also in surface engineering. Shark-skin imitating topographies (parallel riblets with valleys in between) can improve the surface aerodynamics by reducing the drag, and subsequently decreasing the fuel consumption. The selective doping of intermetallic titanium aluminides with fluorine leads to an *in-situ* topography design by influencing the oxidation kinetics of these materials according to the fluorination pattern. Riblets develop on the fluorine free domains and consist of a fast-growing mixed alumina-titania layer. Valleys correspond to the fluorinated regions and, according to the mechanism of a positive halogen effect, are covered by a slow-growing thin alumina layer. The riblet width is first given by the width of non-fluorinated domains and subsequently decreases during high temperature exposure because of the tendency to lateral growth shown by the adjacent mixed oxide. However, the stability of the boundary between mixed oxide and alumina is very important for the maintenance of the aerodynamical improvement.

The minimization of the lateral growth at the junction between mixed oxide and pure alumina depends on the oxide growth rate and the diffusion processes through the different oxides. The investigated samples were first selectively fluorinated by using beamline ion implantation and then exposed to temperatures between 800 and 1000°C. The results refer to the variation of the riblet width for alloys of the second and third generation of intermetallic titanium aluminides. Variations in the oxidation kinetics were induced by changing the temperature or the environment of exposure (i.e. from air to air enriched with 10% water vapor). This paper shows that it is possible to inhibit the lateral growth of the mixed oxide (i.e. riblets) by controlling the temperature of exposure at the very beginning of the oxidation process.

O–TA 22

Investigation on the absorption of fluorine in γ-TiAl and its impact on the oxidation behavior and microstructure

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Due to the high emergence of scrap during the manufacture of γ-TiAl products such as ingot material or final products, a suitable recycling process grants a significant reduction of production costs. The recycling process developed at IME includes an electroslag remelting step which holds the potential to enable a bulk-fluoridation to provide the so called halogen effect. This effect is based on the preferred formation of gaseous Al-halides that are oxidized to Al_2O_3 on the g-TiAl surface which increases the oxidation resistance significantly. As demonstrated earlier the surface doping with fluorine via e. g. ion implantation, gas phase or liquid phase treatment and subsequent oxidation at elevated temperatures leads to the formation of a protective alumina scale for γ-TiAl alloys at temperatures between 800–1000°C.

Thermodynamical calculations using FactSage were performed for the binary alloy Ti-45Al in the presence of F and Ca showing the principal possibility for the fluorine effect at 900 and 1000°C. To investigate the absorption of fluorine in γ-TiAl during electroslag remelting a series of tests was performed. Hence, in a 400 kW lab scale furnace multiple electrodes of the model alloy Ti-45Al were remelted using a CaF_2 based slag. To influence the fluorine absorption and adjust the fluorine content, parameters like melt rate, atmospheric pressure and slag additives were systematically varied. Thereby, a process window was identified wherein fluorine has a positive effect on the oxidation behavior. To review the impact of fluorine, a series of oxidation tests with a variation of temperature (800, 900, 1000°C) and oxidation time (100 and 120 h) was performed.

The samples were analyzed by ESMA and line scans by which a tendency of Al_2O_3 formation and a positive fluorine effect was demonstrated. After isothermal oxidation of 120 h/900°C a tendency to the formation of an Al-rich oxide scale was found. However, this scale is still non-protective. The Al depleted region observed below the oxide scale is a result of a preferred Al
transport to the surface. A Ca-enrichment was found at the metal/oxide interface. The results suggest the tendency to Al_2O_3 formation via a positive fluorine effect. However the F content within the alloy is still too low. Furthermore, the material was examined by non-destructive computer tomography indicating the absence of defects. Microstructure characterization revealed a consistently homogenous fully lamellar α_2/γ-microstructure with different grain sizes dependent on the cooling rate.

O–TA 23

Oxidation behaviour of γ-TiAl alloys coated with intermetallic Ti-Al-Cr based layers

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Intermetallic titanium aluminide alloys are attractive light-weight materials for high temperature applications in automotive and aero engines. Recently, the γ-TiAl alloy Ti-48Al-2Cr-2Nb has been introduced into GEnx™ and LEAP™ engines as low pressure turbine blades. Presently, research and development activities are focusing on γ-TiAl based alloys of the 3rd generation containing the β stabilising alloying elements molybdenum and niobium to increase the service temperature range and to allow component manufacture using conventional hot deformation processing routes. The operating temperatures of these alloys are limited by deterioration in strength and creep resistance at elevated temperatures as well as poor oxidation behaviour above 800°C. Therefore, surface engineering development for protective coatings is an efficient approach to improve the oxidation resistance.

In present work, the oxidation behaviour of coated specimens of the γ-TiAl alloy Ti-48Al-2Cr-2Nb (at.%) and the Mo-containing TNM-B1 alloy was studied performing cyclic oxidation tests at 900°C in laboratory air. The disc-shaped samples were coated with approximately 10 µm thick Ti-Al-Cr-Y and Ti-Al-Cr-Zr layers produced by magnetron sputtering. On both coatings, a continuous thin alumina scale formed. After 1000 cycles of exposure at 900°C (corresponding to 1000 h at high temperature), the yttrium containing coating exhibited a two-phase microstructure of the γ-TiAl and $Ti(Cr,Al)_2$ Laves phases. In the alumina scale as well as in the coating, fine precipitates of the $Y_4Al_2O_9$ phase were observed. The Ti-Al-Cr-Zr coating was composed of an outer layer containing high amount of zirconium and an inner layer with small amount of niobium, being probably $(Ti,Nb)(Cr,Al)_2$ and $(Ti,Nb)(Cr,Al)_2$ Laves phases. Both coatings provided excellent oxidation protection of the substrate materials at 900°C and no spalling of the coatings or oxide scales were observed even on sharp edges.

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O–TA 24

TEM studies of the uncoated and coated Ti-46Al-8Nb specimens after a long-term exposure to air at 700°C

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The objective of this work was to assess the effects of long-term cyclic oxidation on the evolution of microstructure and composition of the near-surface layers of uncoated and coated titanium aluminide alloy, Ti-46Al-8Nb. The overall duration of the test was up to 2000 h, hot-dwell time and temperature were 1 h and 700 °C, respectively. The Cr-Si coatings deposited by magnetron sputtering showed excellent adherence and protective properties. After exposure, the surface was composed of chromium and silicon oxides in the proportions dependent on the initial composition of the coating. Diffusion zone around the alloy/coating interface had an extent of 200-250 nm. For the uncoated alloy, the chemically modified zone resulting from reactive interdiffusion was non-uniform in thickness, from 300 to 1500 nm, depending on the local surface composition of the alloy (γ or a_2 phase). The outermost layer was composed of titanium and aluminium oxides and the inner layers contained titanium nitride co-existing with alumina. Niobium-rich ternary intermetallics were present at the alloy/scale interface. Nanoindentation and scratch tests revealed a significant effect of oxidation and diffusion processes on surface properties of the alloy.

Key words: γ titanium aluminides, oxidation, coatings, TEM

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O–TA 25

Laser-based additive manufacturing – a new processing concept for titanium aluminides

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Additive manufacturing, either using powder-bed processes or direct laser metal deposition, is currently attracting designers and engineers as novel manufacturing technology that widens the limits of conventional manufacturing processes such as casting and forging. While additive manufacturing of titanium alloys, such as Ti-6Al-4V, has matured substantially over the last few year, titanium aluminides are still a great challenge. In order to use the high accuracy and near net shape capabilities of additive manufacturing for TiAl fabrication, appropriate equipment such as inductive heating and an accurate process control and monitoring systems must be applied.

In the present paper, recent achievements of additive manufacturing by laser direct metal deposition using powder of TNM-B1 will be reviewed. Analysis of the raw material as well as the process implementation including downstream processes such as hot isostatic pressing and heat treatment will be reviewed. Taking this into account different microstructures will be considered and compared to the properties of TNM-B1 alloy in as cast plus HIP condition.

O–TA 26

Creep properties of Ti-48Al-2Cr-2Nb produced by selective electron beam melting
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Titanium aluminides have a high potential for aerospace or automotive applications due to their low density and high specific strength. Especially for rotary loads, e.g. in turbine blades or turbocharger wheels, this material class wins over with their high strength-to-weight ratio. The drawback is the difficult manufacturing of this material due to the low toughness and high affinity to oxygen. Selective electron beam melting SEBM, which belongs to the additive manufacturing technologies and works under vacuum conditions, opens a new way of producing complex titanium aluminide parts without significant oxygen pick up and embrittlement. The inherent high cooling rates lead to a very fine microstructure, which was up to now only partly investigated.

In this contribution, the creep properties of SEBM made Ti-48Al-2Cr-2Nb are investigated as a function of the processing parameters. The influence of the building direction on the microstructure and the creep properties is discussed. In addition, the influence of an adequate heat treatment is investigated. The results are compared with results from samples produced by casting.

O–TA 27

Phase distribution in a lamellar Ti-42Al-8.5Nb alloy produced by powder metallurgy
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The addition of niobium to γ TiAl-alloys improves mechanical properties and corrosion resistance compared to their binary counterparts. According to literature the beneficial effect of Nb on mechanical properties lies in modified β and α - transus temperatures that in turn lead to a refined microstructure [1].

In the hot forged ternary γ-Md alloy Ti-42Al-8.5Nb improved high temperature strength and good room temperature ductility were attributed to the occurrence of an additional orthorhombic phase [2]. Detailed investigations by electron diffraction and high-energy x-ray diffraction allowed identification of this phase as O-phase. The orthorhombic O-phase has the ideal composition Ti_2AlNb and has been reported previously in ternary alloys with low Al and high Nb contents in the composition range Ti-(12-31)Al-(12.5-37)Nb [3]. The finding of O-phase in the current alloy is new and implies the need to re-adjust the ternary phase diagram in this composition range.

In the present study the O-phase is identified by single crystal electron diffraction in Ti-42Al-8.5Nb produced by powder metallurgy. The phase forms during low temperature anneal (550°C- 650°C) from α_2 phase. The morphology of phases within α_2 laths of lamellar (α_2+γ) colonies is characterized by conventional imaging techniques, HAADF and high resolution imaging. While the appearance of the modulated α_2 and O-phases resemble martensitic microstructures the sluggish formation during annealing indicates that diffusion plays a role in its formation.

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O–NA 01

The Influence of the Al-concentration on the fracture toughness, hardness and Young's modulus of NiAl single crystals

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B2 NiAl is used as protective coating in various high temperature applications such as turbine blades and vanes in aero engines. The mechanical properties of the stoichiometric NiAl-phase are well established, but the effect of off-stoichiometric composition on the fracture toughness has not yet been systematically studied over the entire composition range of B2 $Ni_{0.5-x}Al_{0.5+x}$. The knowledge of the influence of the Al-concentration in NiAl on the mechanical behaviour, however, is of great importance, because the chemical composition of the coatings changes during service. Here we performed nanoindentation and FIB-milled micro cantilever tests on NiAl single crystals with an oxidation-induced composition gradient to determine the influence of Al concentration on the mechanical properties. While the Young's modulus is found to increase nearly linearly with increasing Al concentration, the hardness displays a minimum at the stoichiometric composition. In the Al rich part of the composition range the hardness increases strongly while it increases moderately towards the Ni rich part. The fracture toughness is maximal for the stoichiometric composition, and plastic deformation accompanies the fracture process for Ni-rich compositions, but not in Al-rich NiAl. Further investigations on the NiAl-phase of bond coats in the as-coated (Al-rich) and thermally cycled (Ni-rich) state were performed and compared with the obtained findings on the binary NiAl single crystals.

O–NA 02

Influence of microstructure on the oxidation behavior of directional solidified eutectic NiAl-X (X = Cr, Mo)

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Nickel aluminide, specifically stoichiometric NiAl (B2 Phase), is a potential candidate to replace Ni-based superalloys in the high-temperature field. The intermetallic compound has a higher melting point (T_m = 1638°C) and is an alumina former which should lead to high oxidation resistance. Additionally, a rather high heat conductivity of 87 $W \cdot K^{-1} \cdot m^{-1}$ combined with a low the density of 5.7 g/cm^3 is beneficial for the use in aerospace applications.

Unfortunately this intermetallic compound suffers from poor room temperature fracture toughness and low creep resistance above 600°C [1]. The introduction of a reinforcing phase in the form of lamellae or fibers, e.g. by directional solidification (DS) of a eutectic, builds a so-called *in-situ* composite material which has been shown to possess both high-temperature strength [2-3] and fracture toughness, while the density is only slightly increased. This second phase will also change the oxidation behavior depending on its size and distribution within the NiAl matrix [4].

In this study, stoichiometric NiAl with different alloy additions of Cr and Mo and nominal compositions of NiAl-33.5Cr-0.5Mo (fibrous) and NiAl-31Cr-3Mo (lamellar microstructure) has been directionally solidified with growth rates varying from 6 to 180 mm/h using a contactless vertical float zone process.

The evolving microstructures, being strongly growth rate dependent, were characterized. The influence on the oxidation behavior is discussed with particular emphasis on the role of fiber/ lamellae properties. Therefore, cyclic oxidation tests at temperatures between 900 and 1100°C for up to 1000 h have been carried out. The oxidation behavior is examined for the NiAl-Cr-Mo alloys and comparatively assessed with fibrous NiAl-Mo [4]. Both Cr-rich alloys exhibit a parabolic mass gain. From the evaluation of the respective parabolic rate constants it is found that the fibrous morphology exhibits a substantially higher scale growth rate at 900°C. The reasons for this finding will be discussed.

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O–NA 03

Study of the hot workability of the directionally solidified fibre-reinforced NiAl-W eutectic alloy

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Constant strain-rate, isothermal compression tests were performed on a directionally solidified NiAl-1.5W eutectic alloy in order to study its hot deformation behaviour and hot workability. The test were conducted in a range of temperatures between 800° C and 1100° C and within the range of strain rates of 10^{-3} – 10^{2} s^{-1}. At high temperature and low strain rates, the flow stress curves exhibited a peak followed by a small drop to a fairly steady state. At the higher strain rate (10^{2} s^{-1}) the flow stress curves showed a cyclic multiple-transient steady state. From the obtained results on the flow behaviour at a strain of 0.1 and 0.5, processing maps were plotted to study the efficiency of the hot working. Instability regions were also pointed out, occurring at all testing temperatures for strain rates higher than 10 s^{-1}. The processing maps identified the highest temperature and lowest strain-rate as the optimum conditions for hot working as expected, with and efficiency of 24%. The activation energy was also calculated in order to obtain the possible active deformation mechanisms. Using a revised constitutive equation it was revealed that the activation energy is not a constant value but it is dependent on the temperature and especially on the strain rate. This behaviour implies that there are two or more active deformation mechanisms active during hot deformation. Microstructure analysis and EBSD maps were conducted to clarify and identify the different mechanisms.

O–NA 04

Micromechanical investigation of the deformation of NiAl-Cr directionally solidified eutectic alloys

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Nickel aluminide (NiAl) has shown great promise for next generation high temperature structural use, due to its excellent properties such as high melting point, low density, high oxidation and corrosion resistance. Low ductility and fracture toughness at room temperature are considered to be restrictions for the use of NiAl, what can be addressed by alloying with refractory metals. Processing alloys with according compositions by directional solidification produces highly aligned eutectic microstructures with enhanced creep properties, fracture toughness and microstructural stability. The alloying addition as well as processing parameters greatly affects the final microstructure and properties of the alloy. Thus, it is important to investigate the mechanical behavior of these materials at varying length scales in order to understand in detail the relationship between microstructure, processing parameters and alloying additions on the macroscopic properties of the material.

The materials for this study have been the eutectic alloy in the NiAl-Cr system, prepared by directional solidification at three different solidification speeds, namely 20 mm/h, 50 mm/h and 80 mm/h, respectively, where NiAl forms the matrix and Cr forms continuous fibers. Fiber diameter and spacing follow an inverse relation with solidification speed and are in the submicron dimension. In order to investigate the dependence of the mechanical properties at room temperature, we have employed different micromechanical testing techniques at various length scales such as nanoindentation, *in-situ* tensile test of individual fibers, and micro-pillar compression tests. Hardness and modulus of overall alloys appear to be independent of the solidification speeds and values for modulus corresponds well with previously reported values. *In-situ* tensile tests of the individual fibers, extracted by chemical etching from the matrix, show that single-crystalline fibers deform plastically up to several percent. For most of the tested fibers, neck formation is observed prior to fracture. Micro-pillars containing single fiber surrounded by matrix as well as single phase NiAl were prepared by focused ion beam milling and compressed with a flat punch in nanoindenter. It is found that pillars with fibers show comparable strength as single phase pillars for similar diameters. Moreover, cross sections across the deformed pillars show no sign of delamination or fracture at the fiber-matrix interface. These results suggest that the fiber-matrix interface is strong enough to accommodate possible mismatch in deformation. TEM examination of the deformed pillars is being carried out to investigate the dislocation mechanisms, and preliminary results indicate that the interface actually acts as a source for dislocation in the NiAl matrix. These observations will be discussed with respect to their impact on the macroscopic fracture toughness and its dependency on the fiber orientation with respect to the loading axis.

O–FA 01

Microstructure refinement in iron aluminide based alloys through industrial processing
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Iron aluminide alloys based on the intermetallic phases Fe_3Al or FeAl are considered for structural applications in harsh environments since long because these lightweight iron alloys show an outstanding corrosion resistance and high wear resistance. As there is no necessity for large amounts of alloying elements and processing with standard equipment readily available at industries is possible, they are an inexpensive alternative to stainless steels or even some Ni base superalloys. While earlier concerns about lack of strength at high temperatures can be overcome by a number of strengthening strategies, limited ductility at ambient temperature still is an issue.

It has been frequently reported that in iron aluminide based alloys ductility can be improved by substantial reduction of the grain size. Therefore the questions arises whether such a grain refinement can be realised through industrial processing and how the obtained microstructures can be preserved during prolonged service at high temperatures.

In a number of ongoing collaborations with industries this question is being pursued. By casting, forging, rolling and additive layer manufacturing (ALM) through selective laser melting (SLM) and laser metal deposition (LMD) various parts have been produced. The microstructures were characterised by light optical and scanning electron microscopy (SEM) including electron backscatter diffraction (EBSD) and mechanical properties are evaluated in the as processed condition and compared to those after prolonged annealing at high temperatures. Partial financial support of this research by the German Ministry of Education and Research (BMBF) under grant 03X3574E and by the regional fond “Rationale Energieverwendung, regenerative Energien und Energiesparen, progress.nrw” of North-Rhine Westfalia and by the Europäischer Fonds für regionale Entwicklung (EFRE), Ziel 2-Programm 2007–2013, Phase VI are gratefully acknowledged.

O–FA 02

Hierarchical microstructure of ferritic superalloys

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A new class of ferritic alloys with hierarchical microstructure is presented, were the bcc-Fe matrix is strengthened by coherent, two-phase $L2_1$-Ni_2TiAl/B2-NiAl precipitates. Electron diffraction, diffraction contrast imaging and aberration corrected scanning transmission electron microscopy (STEM) are applied to study the underlying phase transformation pathways leading to the hierarchical microstructure.

In an alloy with 2 wt.% Ti, spherical B2-NiAl precipitates are forming in the bcc-Fe matrix following rapid solidification. In the course of the aging heat treatment at 700ºC for 10 h the $L2_1$-ordered Ni_2TiAl phase is nucleating exclusively within the B2-NiAl primary precipitates, representing a hierarchical microstructure in terms of chemical ordering and dimension of the phases. The $L2_1$-precipitate substructure adopts a plate shaped geometry with a dimension of 15-20 nm Aberration corrected STEM reveals the coherency with the primary B2-precipitate, a diffuse interface profile and order-disorder fluctuations within the phases.

By increasing the overall Ti content to 4 wt.%, $L2_1$-Ni_2TiAl precipitates are forming in the bcc-Fe matrix after the quench. An internal network of ½<100> antiphase domain boundaries (APB) is revealed within the Ni_2TiAl-precipitates by diffraction contrast imaging. After solid-state aging for 3 h at 700ºC the wetting of initial APBs by the B2-NiAl phase is confirmed using aberration corrected STEM. The B2 wetting layer is growing in width to ~7 nm after aging for 10 h at 700ºC. The interfacial alignment for the corresponding phases is observed to be in a cube-on-cube orientation.

O–FA 03

Effect of ordering on the fracture toughness and creep resistance of Fe-Al-Nb alloys
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An ever increasing demand for materials with excellent high temperature mechanical properties has motivated many researchers to develop intermetallic alloys. Iron aluminides have been considered promising for high-temperature applications, above 700 ºC due to their excellent high-temperature corrosion resistance, good wear resistance and high strength to weight ratio,. This holds true only if their weaknesses such as limited ductility or high temperature strength can be overcome.

Alloying iron aluminides with refractory metals to form precipitates is one approach to improve their brittleness and low toughness. One of the Fe-Al-X systems that has attracted much attention is the Fe-Al-Nb system because of the possibility of strengthening Fe-Al-base alloys by precipitates of either a $L2_1$-ordered Heusler phase or a hexagonal C14 Laves phase. Previous studies have shown that in a Fe-Al-Nb system there is eutectic valley comprising the (Fe, Al, Nb) solid solution matrix and $(Fe, Al)_2Nb$ Laves phase fibers, extending from binary Fe-Nb system almost parallel to Fe-Al side.

In this work, the influence of ordering on the fracture toughness and creep resistance of Fe-Al-Nb alloys was investigated Two alloys containing Laves phase fibers embedded either in a disordered α-(Fe,Al) matrix or DO_3 ordered matrix were investigated in as cast and directionally solidified conditions. Microstructure consisted of either duplex structure of primary dendrites and eutectic (as cast) or fully eutectic structure (directionally solidified). Compression testing showed the yield strength anomaly, which occurred in the 500-650°C range. Alloy with the ordered matrix exhibited higher strength and creep resistance, but lower fracture toughness. The value of stress exponent obtained from the strain rate dependence of the flow stress indicated that the dislocation climb mechanism dominated the creep process. Failure mechanisms were also discussed and related to the microstructure evolution.

O–FA 04

Influence of B on structure and mechanical properties of Fe-Al-Nb intermetallic alloys
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Iron rich Fe-Al based alloys are of great interest due to their outstanding corrosion resistance, low cost of raw materials, high wear resistance, and low density in comparison to stainless steels. However, one of their main disadvantages is lack of strength at high temperatures. Several strengthening mechanisms are available for Fe-Al intermetallics such as solid-solution hardening, stabilization of DO_3 structure, or formation of precipitates, either coherent or incoherent ones. In case of incoherent precipitates, it is desirable that the particles of the strengthening phase are located at the grain boundaries. This distribution is usually not obtainable by conventional solidification. In Fe-Al based alloys, high amounts of alloying elements for the formation of strengthening phases not only increase the prize of the alloy but lead to formation of large Laves phase particles which have no significant strengthening effect. On the other hand, in case of Ta and Nb, addition of only small amounts does not lead to formation of Laves phase but metastable Heusler phase forms instead. In our research, we show that addition of a very small amount of boron changes the solidification kinetics of Fe-Al-Nb, in that instead of metastable Heusler phase the stable Laves phase forms, distributed preferentially on grain boundaries.

In this paper, the microstructure and mechanical properties of Fe-Al-Nb-B alloys with different contents of Nb and Al are described. The microstructure of the alloys was studied by optical and scanning electron microscopy. Mechanical properties were characterized by compression testing at different temperatures and in four point bending. This research is partly supported by the German Ministry of Education and Research (BMBF) under grant 03X3574E.

O–FA 05

Morphology of Fe-Al intermetallic layers evolving in a spark plasma sintering apparatus

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Spark Plasma Sintering / Field Assisted Sintering Technology is an advanced sintering technique, which typically utilizes strong pulsed electrical direct current (DC) to reduce the sintering temperatures and sintering times. In an electrically conductive sample, the pulsed DC induces primarily Joule heating. Furthermore, the applied current is frequently reported to accelerate diffusion processes [1]. Thereby, it modifies the microstructural development as compared to conventional heat treatment methods [2].

In this study, diffusion couples Al-Fe-Al were treated at temperatures between 500°C and 600°C for 30 min to 120 min in order to produce intermetallic phases in the Al-Fe system. This temperature range was connected with the average (root-mean-square) current densities between 64 A/cm^2 and 133 A/cm^2. Scanning electron microscopy including electron backscatter diffraction and transmission electron microscopy were employed to identify the sequence of intermetallic phases and reveal microstructural features in the diffusion zone.

The imposed pulsed DC strongly enhanced the growth kinetics at both interfaces, Al-Fe and Fe-Al. The reaction layers consisted of the intermetallic phases $Al_{13}Fe_4$ (*C*2/*m*) and Al_5Fe_2 (*Cmcm*). The $Al_{13}Fe_4$ phase was not detected after conventional solid state diffusion treatments. The Al_5Fe_2 phase was composed of highly fibre-textured columnar grains that produced strongly fringy Al_5Fe_2 / Fe interface. The crystallographic [001] directions of the Al_5Fe_2 grains deviate less than 15° from the interface normal. A microstructural model has been proposed that describes the origin of the growth morphology of the Al_5Fe_2 phase. It includes microstructural aspects additionally to the previously considered growth kinetics [3].

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O–FA 06

Intermetallic compounds as catalysts for the semi-hydrogenation of acetylene

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Intermetallic compounds offer a wide range of different crystal structures, thus a broad variety of electronic structure scaffolds. Driven by the chemical bonding, a strong site preference and ordered crystal structures result, in contrast to substitutional alloys with randomly occupied crystallographic sites.

In heterogeneous catalysis, the adsorption properties of the corresponding surfaces determine the catalytic properties. In turn, the adsorption strength results from the electronic and crystal structure of the surface. Because of their peculiar combination of crystal and electronic structures, intermetallic compounds represent "new elements" in heterogeneous catalysis. The high stability under reaction conditions and the possibility to vary the chemical potential of the components in a wide range allows addressing fundamental questions.[1]

The semi-hydrogenation of acetylene is an industrially important process to remove detrimental traces of acetylene from the ethylene feed for the production of polyethylene. The catalyst must show high selectivity as well as stability. Polyethylene is the most produced polymer (> 80 Mio. t/a[2]) requiring also very active catalysts. The presence of small and separated transition metal atom ensembles (so-called site-isolation), and the suppression of hydride formation are beneficial for the catalytic performance.[3]

Recent innovation in catalytic semi-hydrogenation is based the experimental realisation of the site-isolation concept employing structurally well-ordered and *in situ* stable intermetallic compounds of Ga with Pd.[4] The stability enables an innovative, knowledge-based development by assigning the observed catalytic properties to the crystal and electronic structures of the intermetallic compounds. Replacing noble metals in heterogeneous catalysts by low-cost substitutes has driven scientific and industrial research for more than 100 years. Cheap and ubiquitous iron is especially desirable, because it does not bear potential health risks like e.g. nickel. Following the knowledge-based approach, the low-cost and environmentally benign intermetallic compound $Al_{13}Fe_4$ was identified as active and selective semi-hydrogenation catalyst.[5]

Besides structural influences, also electronic factors can be determined using solid solutions of intermetallic compounds like $(Ga,Sn)Pd_2$. While all samples in this isostructural series show excellent selectivity - because of the active-site isolation – the activity is strongly influenced by the electron concentration, revealing a maximum at the composition $(Ga_{0.72}Sn_{0.28})Pd_2$. Thus, our innovative strategy based on the use of unsupported intermetallic compounds in catalysis allows a knowledge-based optimization, which was also applied to other heterogeneously catalysed reactions.[6]

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O–FA 07

Iron aluminide alloys modified with selected ternary additions
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Iron aluminides modified with ternary additions (Ta, Nb, Mo or Ti) were produced from elemental powders by self-propagating synthesis (SHS). Products in a form of porous sinters were subsequently arc-melted under argon. The materials were examined in terms of microstructure and phase composition using electron microscopy and standard X-ray techniques (XRD, EDS). Characterization involved room temperature measurements of physical properties and evaluation of corrosion resistance based on electrochemical measurements and/or immersion tests.

Key words: iron aluminides, ternary additions, structure, properties

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O–FA 08

Coarsening kinetics of lamellar FeAl + $FeAl_2$ microstructures in Al-rich Fe-Al alloys
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Fe-Al alloys with about 55 to 65 at.% Al undergo a rapid eutectoid transformation at 1095°C, where the high-temperature phase Fe_5Al_8 (so-called ε phase) decomposes into FeAl + $FeAl_2$. As-cast Fe-Al alloys with about 61 at.% Al reveal a completely lamellar microstructure with average lamellar spacing of about 200 nm. These microstructures resemble those of the well-known $\alpha_2 + \gamma$ lamellar microstructures of Ti-Al based alloys, which are known to result in well-balanced properties in terms of creep, ductility and strength. However, the general properties and the time- and temperature-dependent behaviour of the microstructures is not well known in case of such lamellar Fe-Al alloys.

In this study, a completely lamellar Fe-60.9Al alloy is investigated with respect to the kinetics of lamellar coarsening. Samples of this alloy are heat-treated at different temperatures for different times and, with the help of focused ion beam (FIB) cutting, the true lamellar spacing is analysed by scanning electron microscopy (SEM). The effect of colony size on lamellar microstructure coarsening during annealing also is under investigation. The results are compared to existing models for the growth kinetics of lamellar microstructures.

O–FA 09

Creep properties and microstructure of binary Fe-Al alloys with a fine-scaled, lamellar microstructure

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Fe-Al alloys with an Al content in the range of 55–65 at.% pass through a eutectoid decomposition at 1095 °C, which results in a fine scaled lamellar microstructure (<300 nm lamella spacing) of B2-ordered FeAl and triclinic $FeAl_2$. The lamellar arrangement of the two intermetallic phases may result in an improved creep resistance, which has been already observed for fine lamellar TiAl alloys [1]

Binary Fe-Al alloys with an aluminum content between 58 and 62 at.% were creep tested to evaluate the influence of coarsening kinetics on the creep properties. All alloys exhibit a minimal creep rate in the early stages of creep, which is then continuously increasing with strain. This behavior can be rationalized by the coarsening of the lamella during the creep experiments. Thereby, the creep rate increases with increasing lamellar spacing.

The accurate determination of the lamella spacing requires visualization in three dimensions within a micrograph. Therefore, cross-sections of the samples were milled perpendicular to the surface by FIB to measure the tilt of the lamellae.
To evaluate whether creep stress or strain may contribute to the coarsening kinetics at high temperatures, the alloys were heat-treated without an applied stress and compared to crept samples.

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O–FA 10

Chemically graded iron aluminide – steel samples fabricated by laser metal deposition (LMD)

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Iron aluminide based alloys have been widely investigated because of their interesting properties, i.e. high corrosion resistance to oxidizing environments at relatively high temperature, low density in comparison with stainless steels, excellent wear resistance, adequate strength at elevated temperatures, and low cost of raw materials. The poor ductility of Fe-Al intermetallics at low temperatures, however, hinders widespread structural application. The improvement of ductility has been approached by controlling grain size and morphology. In this respect, additive layer manufacturing (ALM) is a promising method for the production of fine grained materials and it has been successfully employed for processing of Fe-Al alloys [1].

One of the ALM techniques that can be employed to build up complex 3D objects near net shape by using data from a computer-aided design (CAD) file is laser metal deposition (LMD). In this technique a laser produces a melt pool on a metallic substrate, into which continuously powder is fed. By changing the composition of the powder during the built-up process, chemically graded parts can be produced. In case of iron aluminides, parts could be built, which have a higher Al content in areas subjected to corrosion and wear and with a more steel like composition in areas where higher ductility is essential.

In the present work, a number of chemically graded iron aluminide-steel samples has been fabricated by LMD, showing the feasibility to produce such samples. The microstructural changes due to changes in composition were characterized by light optical microscopy (LOM), scanning electron microscopy (SEM), and electron backscatter detection (EBSD). Concentration profiles along the building direction were analyzed by energy- and wavelength dispersive spectrometry (EDS, WDS) and the hardness in dependence of composition has been determined as well. Heat treatments at various temperatures and different times have been performed, to study the long-term stability of the composition gradients. Financial support from the German Ministry of Education and Research (BMBF) under grants 03X3574E/F is gratefully acknowledged

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O–FA 11

Comparison of high temperature oxidation of Fe-40Al coatings obtained by CGS and HVOF

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The objective of the present work is to provide insight into the high temperature performance of iron aluminide intermetallic coatings, sprayed by using High Velocity Oxygen Fuel (HVOF) and Cold Gas Spray (CGS). Initial coating microstructures are compared from the standpoint of the fundamentals of the two techniques. The present results show differences in the oxidation behaviour of the coatings at 900ºC in an oxidizing atmosphere; such differences are especially remarkable for the HVOF coatings when compared to bulk materials because of the highly heterogenous structure. The performance of the CGS iron aluminide coatings is of importance since their direct production by means of cold spray is not straightforward and has not been previously reported; thus, in turn, the report on its oxidizing behaviour is also interesting as a possible alternative to other protective coatings for high temperature applications.

The powder nominal composition is Fe-40Al-0.05Zr (at.%) +50 ppm B. The equipment used for High Velocity Oxygen Fuel (HVOF) spraying process is a Diamond Jet Hybrid (DJH2700) from SULZER METCO, whereas for Cold Gas Spray (CGS), a Kinetics 8000-X prototype (Helmut Schmidt University, HSU) was operated with nitrogen as process and powder feed gas.
Isothermal oxidation tests were performed for 4, 36 and 72 h at 900 ºC in air atmosphere. Once each test was finished, the sample was air-cooled. The microstructural characterization of the feedstock powder as well as the initial and oxidised coatings was carried out by Scanning Electron Microscopy and X-ray diffraction.

The as-sprayed HVOF coatings exhibited the typical features of thermal spray coatings, with the presence of some porosity and oxidation at splat boundaries, which produced the occurrence of some Al-depleted regions. By contrast, CGS coatings resemble to a bulk structure, avoiding any oxidation and porosity, as an inherent characteristic of this solid-state deposition process. Since, the coating is build up through the ability of the feedstock to plastically deform, the difficulty to obtain such coatings comes from the low ductility of these intermetallics.

For the Fe-40Al HVOF coating, the formation of an adherent and fairly homogeneous oxide scale with no cracks was observed, which seems to maintain the same thickness for the three tested periods. It is worth noting that the interface remained intact without appreciable oxidation indicating a good adhesion resulting from the insulating effect of the cement, which permits to determine only the oxidation, which takes place from the contact of the coating surface with the oxidizing atmosphere. A strong diffusion was observed for the cold sprayed Fe-40Al coating but still protection is provided.

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O–FA 12

Comparison of thermal sprayed coatings from iron aluminide powders deposited by HVOF, plasma and flame spray techniques on an Al-Si-alloy

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Due to their good mechanical properties and outstanding corrosion and oxidation resistance at higher temperatures iron aluminides provide promising potential for applications at elevated temperatures. Their relatively low density together with low costs and wide availability of their raw materials coupled with good tribological attributes are attractive aspects to think about corrosion-, oxidation- and wear protective coating materials. Several investigations were carried out in the past to apply iron aluminides by use of different thermal spray techniques on steels as oxidation- and wear protective coatings. Another field of application could be the utilization of iron aluminides as thermal barrier coatings on hypoeutectical aluminum-silicon alloys. Due to their notably lower thermal conductivity of B2- and $D0_3$-ordered Fe-Al alloys in comparison to Al-Si alloys these materials exhibit a great potential. Furthermore these two material systems have similar coefficients of thermal expansion which can be varied by the amount of aluminum in the iron aluminides. Therefore, gas atomized Fe-Al-Cr powders were applied by the thermal spray techniques atmospheric plasma spraying (APS), flame spraying (FS) and high-velocity-oxygen-fuel spraying (HVOF) on Al-Si substrates and the coatings´ microstructures were investigated. Phase analyses were performed using XRD and SEM combined with EDX-measurements which identified different solid solution, intermetallic and oxide phases. Pore distributions as well as microhardness of differently produced coatings were compared. The adhesive tensile strength of these coatings was determined using standardized tensile pull-off tests and the cracking behavior was observed by performing bending tests. Isothermal heat treatments at temperatures up to 500°C were used to qualify the thermal stability of these coatings.

O–SA 01

Physical simulation of investment casting of nozzle guide vanes made of Ni-based superalloys
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Development of investment casting process has been a challenge for manufacturers of complex shape parts. Numerous experimental casting trials are typically carried out to determine the optimum casting parameters for fabrication of high quality products. Here, we present a new tool for physical simulation of investment casting that can accurately predict microstructure and hardness in as-cast complex shape parts. This physical simulation tool consists of a thermal model and melting/solidification experiments in a thermo-mechanical simulator. The thermal model is employed to predict local cooling rate during solidification at each point of a casting. Melting/solidification experiments are carried out under controlled cooling rates determined by the thermal model. Microstructural and mechanical characterization of the solidified specimens is performed and databank on the effect of cooling rate on the microstructure and mechanical properties is generated. Thus, the local microstructure and local mechanical properties can be accurately predicted at each point of casting.

This concept is applied to investment casting of complex shape nozzle guide vanes (NGVs) from a Mar-M247 Ni-based superalloy. Experimental casting trials are performed, temperature history of metal and ceramic shell during experimental casting is recorded, and the thermal model is validated against experimental results. The outcomes of thermal model, i.e. local cooling rates during solidification of the NGVs, are used as input parameters for melting/solidification experiments in the GLEEBLE 3800 thermo-mechanical simulator. The samples after melting/solidification experiments in the GLEEBLE system are subjected to detailed microstructural characterization. It is demonstrated that phase composition, secondary dendrite arm spacing, grain size, γ/γ´eutectic size and volume fraction, size and shape of carbide particles, and local microhardness are very well predicted at each point of the casting via physical simulation. The advantages of application of physical simulation tool for development of novel casting routes are discussed.

O–SA 02

Orientation relationships and phases in Co-Al-W alloys
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TEM study of the equilibrium intermetallic phases and structure evolution in Co-Al-W alloys are presented. Co-9at.%Al-Xat.%W alloys containing different ordered phases have been investigated. The features of the crystallographic transitions and orientation relationships between the equilibrium phases like: γ (FCC), Co_3W ($D0_{19}$), Co_7W_6 (μ-phase, $D8_5$), CoAl (B2), and $Co_3(Al,W)$ (γ'- $L1_2$) in Co-Al-W alloys are found. The lattice mismatch of γ'/γ and elastic coherency strains are calculated. The modulated structures formation and the spinodal decomposition in Co-base systems with a limited solubility of alloying elements are discussed.

O–SA 03

Effect of ordering on hydrogen affected dislocation behavior in Ni-Cr superalloys

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In severe corrosive or high temperature environments, such as chemical plants and deep sour gas fields, Ni-base superalloys have often been used because of their excellent corrosion and heat resistance. During long-term exposure at high temperatures, however, Ni-based alloy occasionally undergo microstructural changes due to the formation of Ni_2Cr, Ni_2Mo, and $Ni_2(Cr,Mo)$, which are ordered orthorhombic (oI6) phases. The present studies have investigated the ordering behavior from single phase fcc to oI6 phase in Ni-Cr binary alloys and commercial Ni-Cr-Mo-W alloys. TEM observations have indentified the super-diffraction spots, which represent short-range-ordering and long-range-ordering after aging at 773K. High contrast TEM observations of lattice image in aged specimen have shown that the long-range-ordered specimen consists of fine ordered domains less than 10nm in diameter. However, the ordering has been suppressed in quenched specimens, which were solution treated at high temperatures and followed by water quenching. In the commercial alloy, substituting Mo or W for a part of Cr has also retarded the formation of ordered phase. Electronic structure calculations have suggested that the ordering kinetics is controlled by vacancy and substitutional atoms.

The effect of ordering on mechanical properties has been investigated by means of tensile tests with hydrogen charging to evaluate strength, ductility, and susceptibility to hydrogen embrittlement. The yield strength and work hardening rate were increased more than twice by ordering without a reduction in tensile elongation. Although, the susceptibility to hydrogen has reduced during the short-range-ordering, the long-range-ordering has enhanced hydrogen embrittlement. The hydrogen embrittlement in the Ni-Cr and Ni-Cr-Mo-W alloys has been characterized by a fracture mode and deformation structures. The fracture mode due to hydrogen embrittlement has changed from intergranular fracture to transgranular fracture, which propagates along to deformation twin boundaries, with increasing the degree of order. The dislocation in the ordered specimens is characterized by super-dislocations, which consist of three parallel dislocations separated by anti-phase boundaries. The tensile tests in Ni-Cr single crystal have suggested that the hydrogen charging has activated super-dislocations enough to induce deformation twinning in small stress. It will be discussed the effect of hydrogen on the plasticity of ordered phase.

O–SI 01

Environmental/thermal barrier coating systems for Nb/Nb_5Si_3-based high-temperature alloys

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Nb/Nb_5Si_3-based alloys are potential high-temperature materials for turbine engine applications at temperatures up to 1300°C. However, their oxidation resistance is poor and, therefore, oxidation protective coatings as well as environmental/thermal barrier coatings (E/TBCs) are required to protect these materials against environmental attack in gas turbine combustion atmospheres.

In this study, E/TBC systems of yttria partially stabilized zirconia (YSZ), gadolinium zirconate (GZO) and a combination of Y_2SiO_5 and $Gd_2Zr_2O_7$ were applied on Nb-Si based alloys. An FeB-modified M_7Si_6-based bond coat produced by pack cementation was used. The YSZ and GZO topcoats with thicknesses in the range between 150 and 200 µm were deposited on one side of rectangular coupons using electron-beam physical vapor deposition. Furthermore, a combined E/TBC of yttrium silicate and GZO was applied with a 15–20 µm thick Y_2SiO_5 layer manufactured by magnetron sputtering. The lifetimes of the different E/TBC systems were determined performing cyclic oxidation tests at 1100°C and 1200°C in laboratory air (exposure at high temperature for 1 h followed by 10 min forced air cooling at ambient temperature). Post-oxidation cross-sectional examinations were carried out using scanning electron microscopy and energy-dispersive X-ray spectroscopy.

The E/TBC systems exhibited lifetimes exceeding 1000 cycles when exposed to air at 1100°C. The ceramic topcoats were well-adherent to the thermally grown oxide scales; and the remaining bond coat protected the substrate against oxidation. At 1200°C, lifetimes approaching 1000 cycles were determined. However, substantial material recession was observed with prolonged thermal cycling testing, caused by oxide spallation at the edges and rear side of the samples (areas without E/TBC). In the sample's center area, the E/TBC systems were still intact.

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O–SI 02

Determining the eutectic point of Mo-rich Mo-Si-B alloys

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Ni-based superalloys have been extensively used as high temperature materials in gas- and aircraft turbines for decades. However, the well-known thermal instability of the γ/γ' microstructure limits the applied surface temperatures to a maximum of around 1150°C. Consequently, new high temperature materials must be developed to further increase the efficiency of these thermal aggregates like for instance turbines.

The present work addresses Mo-Si-B alloys of the Mo-rich region of the phase diagram, which are located in the so-called "Berczik triangle". These alloys consist of a three-phase microstructure with a Mo solid solution phase (Mo_{SS}) and the two intermetallic phases Mo_5SiB_2 (T2) and Mo_3Si. Different alloy compositions in the respective primary solidification areas of the Mo_{SS}, T2 and Mo_5Si_3 phases were chosen to investigate the microstructural evolution. The alloys were produced by arc-melting and investigated using SEM-BSE images and EPMA measurements. The results were compared to thermodynamic calculations of the liquidus projection and isopleth phase diagrams using the software FactSage™. By carrying out these experiments it was possibly to determine the ternary eutectic point, which was found to have a nominal composition of Mo-17.5Si-8B (at.%). The ternary eutectic composition is expected to combine properties such as high strength and an excellent creep and oxidation resistance of Mo-Si-B alloys.

In a second step the ternary eutectic composition was chosen for a directional solidification process (DS), since it is known from the literature that eutectic compositions may result in a well-defined microstructure with lamellar or fibrous morphologies using DS. In agreement with the solidification pathway a ternary eutectic DS alloy Mo-17.5Si-8B could be achieved which showed well-aligned ternary eutectic colonies parallel to the growth axis. Additionally, the mechanical properties of the eutectic alloy composition had been tested in terms of indentation fracture mechanics and compressive creep strength in the temperature range from 1100-1400°C. The results of the creep tests were evaluated and compared with a commonly used Ni-based superalloy, the arc-molten Mo-17.5Si-8B eutectic composition and a powder metallurgical (PM) processed alloy Mo-9Si-8B. The eutectic cast and DS Mo-Si-B alloys possess a superior creep resistance showing great potential for applications at temperatures of around 1200-1300°C.

O–SI 03

Directional solidification of ternary Nb-Si-Cr eutectics and its influence on the creep behavior

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Niobium silicide based alloys are promising materials to replace Ni-based superalloys in high temperature structural applications due to their high melting point and comparably low density [1]. Unfortunately, good mechanical strength and oxidation resistance at elevated temperatures are difficult to be achieved simultaneously in a satisfying manner.

Our approach is that this challenge may be met by directional solidification (DS) of eutectic alloy compositions. Whilst DS processing can lead to enhanced creep lifetimes by minimizing the amount of transversal grain boundaries within the material [2], eutectic alloys have been shown to positively alter the creep properties due to the formation of a continuous and fine lamellar microstructure [3].

For this reason, the eutectic composition of the ternary system Nb-Si-Cr is directionally solidified employing a vertical float zone process. In this system, silicon is known to significantly improve the creep properties by formation of silicide phases (e.g. $Nb_9(Si,Cr)_5$), whereas chromium is added to mainly improve the oxidation resistance due to the potential for Cr_2Nb Laves phase formation [4]. The influence of varying processing parameters (growth rate, rotating speed and direction of the feed and seed rods) on the resulting microstructures is comparatively assessed. Compressive creep tests in vacuo under constant stress at temperatures up to 1300°C give insights into acting creep deformation mechanisms. First results indicate dislocation creep to be present, leading to an increased creep rate as compared to the DS binary eutectic Nb-18 at% [5]. This results from the presence of the comparatively weaker Cr_2Nb Laves phase, in which the presence of dislocations was observed by means of TEM also. Moreover, in comparison with arc-molten samples of the same ternary composition, the potential of the DS eutectic to improve mechanical properties at elevated temperatures is assessed. Surprisingly, first results show a superior creep resistance of the arc-molten samples, even though their microstructure is not aligned and much finer in terms of phase size. We will try to shed light onto this observation.

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O–SI 04

Interface structures in directionally solidified $MoSi_2$ / Mo_5Si_3 / Mo_5Si_3C eutectic composites

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One of the possible ways to improve the poor fracture toughness of monolithic $MoSi_2$ is to form composites with other hard materials. $MoSi_2$ / Mo_5Si_3 eutectic composite with high eutectic temperature (1900°C) is a promising candidate since the improvement of the fracture toughness is expected to be possible through controlling their interface properties. Recently, we have systematically studied the influences of ternary addition on microstructure and mechanical properties of directionally solidified $MoSi_2$ / Mo_5Si_3 eutectic composites with the so-called script lamellar structure and confirmed that the interface fracture behavior can be modified by controlling the lattice misfits or interfacial segregation. In addition, there is a further probability to control the interface properties by introducing an additional phase into the $MoSi_2$ / Mo_5Si_3 script lamellar structure. In the present study, orientation relationships and interface structures in directionally solidified $MoSi_2$ / Mo_5Si_3 / Mo_5Si_3C eutectic composites were investigated by electron backscatter diffraction (EBSD), atomic resolution scanning transmission electron microscopy (STEM) and transmission electron microscopy (TEM). Mo_5Si_3 and Mo_5Si_3C phases individually form interconnected networks in the $MoSi_2$ matrix, maintaining the [1-10] of $MoSi_2$, [001] of Mo_5Si_3 and [0001] of Mo_5Si_3C approximately parallel to the growth direction. The orientation relationships between $MoSi_2$ and Mo_5Si_3 in the three-phase composites are confirmed to be identical to those in the two-phase composites. Atomic scale investigations of the various interfaces confirm that the Mo_5Si_3 / Mo_5Si_3C interfaces possess relatively high coherence compared to the $MoSi_2$ / Mo_5Si_3C interfaces, implying that the latter interfaces exhibit a higher probability of interface delamination.

O–SI 05

Bond coat alumina forming intermetallic alloys for coatings for Nb silicide alloys

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Niobium silicide based alloys, like the Ni based superalloys, will require coating system for use in high temperature structural applications in future aero-engines. Coating systems of the bond coat (BC)/thermally grown oxide (TGO)/top coat (TC) are currently considered. The coating system should have capabilities of TBCs used on Ni based superalloys but should also offer protection of the substrate from interstitial contamination.
Multi-alloy or functionally graded BCs capable of forming alumina TGO are highly desirable for coating systems for Nb silicide based alloys. The presentation will discuss design criteria for multi-alloy or functionally graded BCs and for selecting intermetallic alloys (i) suitable for use in such BCs, and (ii) capable of forming continuous α-Al_2O_3 scales. Examples will be discussed and results will be compared with available data.

O–SI 06

The oxidation behaviour and crystallographic features of single phased $(TT'Cr)_7Si_6$ silicides (with T = Nb and Ti and T' = Fe, Co, Ni)

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Among the coating possibilities to protect niobium silicide *in-situ* composites against high temperature oxidation, silicides are likely one of the most promising way. Complex silicide coatings were developed based on the Fe-Cr-Si and Ti-Cr-Si ternary phase diagrams. One type of silicide, the $(TT'Cr)_7Si_6$ phase (with T=Nb and T'=Fe) having the $P4_2/mbc$ space group, exhibits very high oxidation resistance at high temperature and was successfully deposited at the surface of the NbSi composite by using the pack-cementation process [1,2].

In the present work, modifications of the composition of the $(TT'Cr)_7Si_6$ were performed in order to study the oxidation resistance of single phased compounds. Six compositions were prepared by substituting Nb for Ti and Fe for Co and Ni. Their full characterization by SEM and XRD highlighted that the nature of the T' metal only had an influence on the compositions. Indeed, such changes did not modify the crystal structure of the $(TT')_7Si_6$ [2] but affect thechromium content into the silicide.

Isothermal oxidation studies at temperature as high as 1300°C evidenced very low degradation rate for all compounds. All phases developed a duplex protective oxide layer composed of chromia and silica. It was found that the ratio chromia/silica depends on the nature of T'. The oxidation study also evidenced enhanced chromium diffusion in Ni containing silicides but did not induce phase transition.

In the present paper, these results will be discussed regarding the crystal structure and the position of Cr atoms assessed by theRietveld refinement method.

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O–SI 07

Effect of Si concentration on the properties of V-Si solid solution powders

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With this work a contribution to the development of new vanadium-based materials as light-weight high temperature materials should be made. Metallic alloys and compounds which provide a high melting point and enhanced high temperature resistance are of special interest and more topical than ever. Several new alloys based on elements with ultra-high melting points like molybdenum (T_m = 2623°C) and niobium (T_m = 2467°C) are currently under development and investigation. Compared to the materials mentioned above, vanadium was identified as a high potential candidate since it provides the lowest density (ρ = 6,11 g/cm^3) of high melting point metals (T_m = 1910°C). In the present work investigations on solid solution effects in V-Si alloys, to create a reference for three-phase V-Si-B alloys, will be presented. Si appears to be an effective solid solution strengthener for V and leads to an improved hardness due to the solid solution strengthening effect. Therefore, the influence of the Si concentration, ranging between 2 and 25 at.%, on high-purity V(Si) solid solution materials produced by mechanical alloying was investigated by microstructural characterization using SEM in combination with FIB preparation and XRD. The mechanical behavior of the powder samples was analyzed using micro hardness measurements. the solid solution strengthening effect, the mechanical alloying process affects a reduction of the grain size as well as strain hardening due to the applied impact energy during ball milling. To estimate the influence of these aspects Williamson-Hall analysis had been implemented.

O–FU 01

Temperature dependence of mechanical properties of the $Fe_{81}Ga_{19}$ (Galfenol) alloy

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Mechanical properties of most metals or alloys are anelastic (i.e., not ideally Hookeian). The $Fe_{81}Ga_{19}$ (Galfenol) alloy is no exception. Besides, the $Fe_{81}Ga_{19}$ alloy is ferromagnetic below its Curie temperature (T_C), about 713°C. Mechanical properties, such as the Young's modulus (E), shear modulus (G), damping capacity (ΔW/W), were measured by the impulse excitation method under the following two conditions: [1] temperature (T) varied from room temperature (RT) to 300°C, and [2] external magnetic field (H) changed from 0 to 200 Oe. In the E vs. T plot (when H = 0), there is a downward kink at $T = T_{mF}$ = 232°C, which indicates that when $T < T_{mF}$, we have the un-relaxed Young's modulus (E_U), and when $T > T_{mF}$, the relaxed Young's modulus (E_R). The anelastic (or non-magnetic) ΔE effect (near T_{mF}) is defined as $(\Delta E)_{AN} = [E_U – E_R]/E_R = 0.46\%$. In turn, in the E vs. T plot (when H = 200 Oe), there is almost no kink at T_{mF}, which implies the off-set due to the magnetic ΔE effect: when $T < T_{mF}$, $(\Delta E)_{HU} = [E_{HU} - E_U]/E_U$ and when $T > T_{mF}$, $(\Delta E)_{HR} = [E_{HR} - E_R]/E_R$. Since the situation is no kink when H = 200 Oe, we believe that $(\Delta E)_{HR} > (\Delta E)_{HU} > 0$ near T_{mF}. The Debye peak $(1/Q)_F = ([1/2\Pi][\Delta W/W]_F)$ at constant flexure resonance frequency (f_{RF} = 1830 Hz) can be plotted as a function 1/T. From this plot,[1,2] we can determine the activation energy (E_A) for domain wall motion in the alloy: E_A = 0.436 eV/atom. At T = RT, the saturation field (H_S) is about 3 KOe for the magnetic ΔE and ΔG effects: the former is $(\Delta E)_{HR}$ = 5.23%, and the latter is $(\Delta G)_{HU} = [G_{HU} - G_R]/G_R$ = 5.39%. The downward kink in the G vs. T plot (when H = 0) occurred at $T = T_{mT}$ = 199°C.

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O–FU 02

The nano-crystalline superelastic NiTi intermetallic – the effect of heat treatment on the structural, mechanical and corrosion characteristics

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NiTi intermetallics show superelastic behavior, shape memory effect, high corrosion resistance and a relatively good biocompatibility making them of interest for medical implant applications. Severe cold plastic deformation can be used to prepare ultra-fine-grained or nano-crystalline alloys.

In the presented contribution, the nano-crystalline Ni-Ti (50.9 at. % Ni) intermetallic was prepared by cold drawing. Various short-time heat treatment regimes at 300–600°C were applied subsequently to simulate technological steps in the manufacture of medical implants like stents. Microstructure, mechanical properties and corrosion behavior of the heat-treated material were investigated by using SEM, TEM, XPS, hardness, tensile, fatigue tests and immersion corrosion tests. The observed characteristics were related to the regime of heat treatment. It was demon strated that the nano-crystalline structure, mechanical properties and corrosion resistance of the material remained stable up to 300°C. At above

this temperature all the material characteristics changed siginificantly. Structural modifications involved grain growth and precipitation of new intermetallic phases which resulted in significant hardening of the material. Heat treatments also induced modifications of the surface structure of the material leading to an unfavourable decrease of the corrosion resistance. The observed behavior of the NiTi intermetallic was discussed in terms of current medical applications.

O–FU 03

Correlation between electrical resistivity and phase intermetallic structure in the 3D porous SMA synthesized during SLS/M process

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Presence of shape memory effect (SME) in porous biocompatible materials, synthesized layer-by-layer via selective laser sintering/melting (SLS/SLM) method, and possibility of laser additive manufacturing (LAM) of 3D bio-MEMS (i.e. implants, sensors, drug delivery systems etc.), are new quality level which can be achieved in medical applications through development of self-initiating,, self-fixing, and self-swinging prosthetic elements at a living tissue.

In the present work, we demonstrate how LAM technology can contribute to a better understanding of functional and structural properties of shape memory alloys (SMAs) in Ni-Ti and Cu-Al-Ni systems. Correlation of specific resistance and phase structure in porous nickel-titanium and CuAlNi intermetallic phases after LAM was experimentally observed. It was shown, that electrical resistivity of the phases studied (austenite, R-phase, martensite) increases with temperature but the slopes are quite different. Intermediate R-phase in nitinol (NiTi - intermetallide) shows generally higher electrical resistivity than the austenite phase, but its value grows with the decrease of temperature for SLS samples. We explained this fact by accumulation of dislocation with the continuous increase of the R-phase with the decrease of temperature. No similar dependence was observed for the SLM samples. Hysteresis loop of the electrical resistivity is more remarkable in SL-Sintered samples than in SL-Melted samples due to different 3D part's porosity and is a lot higher then that of the solid material of similar composition.

O–FU 04

Ferromagnetic shape memory alloys

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Since its discovery in 1932 and explanation in early 50s shape memory alloys (SMA) came a long way. They became applied in various industries even in medicine in the form of stents and other implants. Except application based research, the investigation of SMA helps to understand various aspects of martensitic transformation. Early 90s brought (again) the attention to magnetically induced martensitic transformation in ferromagnetic SMAs and particularly Ni-Mn-Ga(In) based alloys formed new topic. Apart of magnetically induced transformation there is another effect called magnetically induced reorientation (MIR) of martensitic structure [1]. Thanks to this effect the off-stoichiometric Ni_2MnGa alloys exhibit length change about 12% in the magnetic field below 1 T [2]. The low-temperature martensitic structure of Ni-Mn-Ga is unusual with various types of the modulation of basic 2H structure. Up to now the crystallographic description of these structures are not settled and recent investigation suggests the probabilistic stacking of nano-twinning boundaries creating just effective elementary cell (it may be similar surprise as it was the boundaries mobility in iron-aluminides presumed by Hilfrich and Nembach [3]). Compared to Ni-Mn-Ga system with various modulations and extremely low energy of twinning boundaries, the ferromagnetic shape memory Co-Ni-Al systems exhibit just B2 to $L1_0$ transformation without modulation and the martensite transformation or the reorientation could not be induced by magnetic field [4]. However, the stress induced transformation is available at wide temperature range [5]. In contrast to Ni-Mn-Ga the wide variety of nanoprecipitate types are observed in Co-Ni-Al alloys similar to Ni-Ti alloys [6]. These nanoparticles are thought to be responsible for deformation via twinning as the long-distance force fields of precipitates block the moves of dislocations. On the other hand, no such precipitates were found in Ni-Mn-Ga and no high dislocations density observed presumably due to high energy formation in ordered structure, which leaves the twinning as the favorite way of deformation also in Ni-Mn-Ga.

In the presented lecture we try to compare functional properties of both systems with their microstructure. We expect here crucial role of twinning boundaries, high-temperature order and, if any, formation of nanoparticles. It seems that these systems can be understood as the model types of SMAs.

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O–FU 05

Phase stability of intermetallic compound in Cu-Mn-Al and Cu-Ni-Al alloys and industrial applications

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The Heusler phase in the Cu-Mn-Al system is well known and $L2_1$-B2-A2 order-disorder transition occurs in a wide range of compositions. Based on this ordering behavior, superelastic alloys with a low degree of order characterized by high ductility, high cold workability and good machinability have been developed. Such an alloy has been used for an ingrown nail correction device[1], which has been used in more than 2500 hospitals in Japan. Since the superelastic property is affected by the microstructure, a large grain size is required to obtain a high superelastic strain[2]. Recently, a large grain structure has become obtainable by special heat-treatment[3], which allows production of a superelastic bar with high recovery strain in industrial plants. Such bars are expected to be applied in seismic control structures as reinforcement elements in concrete beams and braces, as well as for rehabilitation of clay-unit masonry walls and so on[4].

Furthermore, Cu-Ni-Al-based alloys with high strength and high electronic conductivity were designed using a thermodynamic database of Cu-based alloys including the elements Cu, Al, C, B, Cr, Fe, Mn, Ni, P, Si, Sn, Ti and Zn. These new alloys have been strengthened by the $(Ni, Cu)_3Al$ phase with an $L1_2$ structure and are being commercially produced for suspension wire in a DVD device.

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O–ST 01

Al-Fe-Ni-Ti Calphad state of the art

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The Al-Fe-Ni-Ti system is of high interest for different kind of structural materials like superalloys, maraging steels, titanium alloys, titanium aluminides, iron aluminides, memory shape alloys. This system exhibits the stability of different intermetallic phases showing ordering relationship with solid solutions like in the fcc familly the $L1_0$ (AlTi) and the $L1_2$ (Ni_3Al, Ni_3Fe) phases, in the bcc familly the B2 (AlFe, AlNi, NiTi, FeTi), the DO_3 (Fe_3Al), the $L2_1$ ($AlNi_2Ti$, $AlFe_2Ti$ or in the hcp familly the DO_{19} (Ti_3Al). The thermodynamic description of these phases considering this relationship is the way to built databases of quality for more complex compositions. The status of the art of Calphad description in this quaternary system will be presented.

O–ST 02

Thermodynamic study of the Nb-Ru-Al ternary system: experimental and Calphad approaches

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Nb-based alloys are candidates for replacing currently used Ni-base superalloys in high temperature applications because of their low densities, high melting points and high strength. However, their poor oxidation resistance has been a major barrier to their practical applications. As a satisfactory balance between mechanical properties and oxidation resistance at high temperatures has not yet been achieved by alloying elements, a protective coating is necessary for their use at high-temperature in oxidizing environments.

Niobium silicides are widely involved as coating materials, but simple binary niobium silicide coatings have limited oxidation resistance. Therefore, many studies have been carried out to develop modified silicide coatings mainly by using the halide activated pack cementation technique (HAPC). However, there are fewer reports in the open literature about efficient aluminide coatings capable to protect Nb-based alloys through a long term adherent alumina.

Thus, the purpose of the present study was to perform the thermodynamic assessment of the Nb-Ru-Al system which should be useful *in fine* for determining the conditions of HAPC leading to the deposition of an innovative alumina-forming coating. Indeed, preliminary results show that i) Ru can act as a barrier against the diffusion of Al into the niobium substrate [1] and ii) $RuAl_{1-x}Nb_x$ should constitute a stable Al reservoir promoting the well known protective Al_2O_3 scale [2].

The obtained outstanding results are: (i) the study of Nb-Ru section reveals the existence of a 2nd order transformation (Nb, Ru) -A2 / B2, the $NbRu_2$ compound whose crystallographic structure was determined by anomalous diffraction using synchrotron radiation, a Calphad modeling was performed, (ii) the Nb-Ru-Al diagrammatic data related to the isothermal section at 1100°C are well restituted by the CALPHAD modeling, (iii) the liquid projection was experimentally investigated.

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O–ST 03

High entropy silicide composites? What are the rules for designing their high entropy solid solution phase?
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Nb silicide based alloys (or Nb *in situ* silicide composites) have the potential to replace Ni based superalloys in high temperature engineering applications. The two most important phases in the microstructure of these new alloys are the bcc Nb solid solution (Nb_{ss}) and the tetragonal Nb_5Si_3 silicide. Different types of solid solution can form in these new alloys. The Nb_{ss} is the key phase for Nb silicide based alloys meeting and exceeding property goals.

Alloying with transition metals, including refractory metals, and with simple metals and metalloids is essential for improving the mechanical behaviour and oxidation of the Nb_{ss}. Two questions (among many others) that are critical for designing Nb silicide based alloys are: (a) what are the rules that determine (govern) the formation of the bcc Nb_{ss} in Nb silicide based alloys? (b) can the bcc Nb_{ss} in these alloys be (or made to be) a "high entropy alloy" (HEA) solid solution of the type reported for bcc solid solution HEAs?

The presentation will confirm (b) in alloys that are classified as High Entropy Matrix Silicide Composites(HEMSiCs) or Silicide Matrix High Entropy Composites(SiMHECs). The presentation also will (i) discuss the different types of Nb_{ss} that can form in these materials, (ii) present and discuss the rules that favour the stability of different forms of the Nb_{ss}, and (iii) link solid solution hardening with rules for solid solution formation in these materials.

O–ST 04

Interactions of liquid Au-Si with Cu, Ni and Ti – phase equilibria and new ternary compounds
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The extremely deep eutectic in the Au-Si system (363°C at 19 at.% silicon) attracted much attention from the basic as well as from the application point of view. Potential applications include Au-based bulk metallic glasses for jewellery applications, the synthesis of silicon nanotubes, and the joining of components for micro- and nano-electro mechanical systems. In the current work, the equilibrium phase diagrams Au-(Cu,Ni,Ti)-Si have been studied, as interactions of liquid Au-Si with copper and nickel and titanium substrates are of potential interest for joining applications, e.g. in electronics.

The ternary systems were studied by a combination of powder X-ray diffraction, scanning electron microscopy and DTA. Several new ternary compounds have been synthesized and structurally characterized by single crystal XRD: $Au_{5\pm x}Cu_{2\pm x}Si$ (*Pnma*, *oP*32) shows an extended homogeneity range, while $AuNi_3Si_6$ (*R*-3m, *hR*30), $Au_2Ni_4Si_7$ (*C*2/*m*, *mC*26) and $Au_{10}Ti_9Si_6$ (*Cmca*, *oC*50) are stoichiometric compounds. All ternary compounds are crystallizing in new structure types. The ternary systems were investigated for several isothermal sections, with special emphasis to low temperature phase equilibria close to the binary Au-Si eutectic. Partial ternary reaction schemes and liquidus surface projections for the three systems were derived from DTA data.

O–ST 05

Modelling topologically close-packed phases in superalloys and steels

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Topologically close-packed (TCP) phases play an important role in many modern alloys and steels. While particular TCP phases are desirable in precipitate-hardened steels, the precipitation of TCP phases in single-crystal superalloys has a detrimental effect on the mechanical properties. In order to gain a microscopic understanding of TCP phase formation, we investigate the factors that drive their structural stability. In particular, we employ electronic-structure calculations at different levels of coarse-graining, ranging from density-functional theory (DFT) to tight-binding to analytic bond-order potentials (BOPs). We demonstrate that the role of electron count on the trend of structural stability of TCP phases across the transition-metal (TM) series can be identified on all levels of coarse-graining. The interplay of electron count and size-mismatch as dominating factors for the stability of TCP phases is analysed by comparison of DFT calculations for various binary and ternary TM alloys to an empirical structure map. This structure map is further applied in a concerted effort with casting experiments and microstructure analysis in order to provide guidance for the analysis of TCP phase precipitates.
In particular we show that the combination of the structure map with experimentally determined local chemical composition enables to identify TCP phase precipitates in Co-based and Ni-based superalloys.

O–ST 06

Thermodynamic modelling at low temperatures – Combined *ab initio*, semiempirical and experimental approach

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In thermodynamic modelling above room temperature, the Gibbs energy of elements is well described in the SGTE database [1] and this description is based on experimental data. However, below room temperature, any unified description of thermodynamic functions is missing. In general, at low temperatures, the heat capacity can be described principally correctly by Einstein function [2]. In this approach, the Einstein temperature (T_E) plays the role of fitting parameter and can be taken from literature. Nevertheless, for some elements (e.g. for Pb, Cd), the literature data for T_E do not allow us to extend the heat capacity below room temperature smoothly [3]. T_E can also be determined from the experimentally found or *ab initio* calculated temperature dependencies of heat capacities in the low-temperature region. The electronic and anharmonic contributions are then adjusted to provide continuous connection of heat capacities and Gibbs energies between low-temperature and high temperature region. In the presentation we show our way of determination of T_E, the low-temperature evaluation of Gibbs energies and heat capacities of selected phases and some low-temperature phase diagrams. Our heat capacities in low-temperature region calculated from first-principles are also presented.

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O–ST 07

Supersaturated intermetallic phases within the ternary Mo-Cr-N system

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Although many research activities concentrate on transition metal nitrides, due to their excellent properties, only little is known for Mo-N based materials. We investigate in detail the influence of Cr on the structural evolution and mechanical properties of Mo-N coatings prepared at different nitrogen partial pressures. The chemical composition as well as the structural development of coatings prepared with N_2-to-total pressure ratios (p_{N2}/p_T) of 0.32 and 0.44, can best be described by the quasi-binary Mo_2N-CrN tie line. Mo_2N and CrN are face centred cubic (fcc), only that for Mo_2N half of the N-sublattice is vacant. Consequently, with increasing Cr content also the N-sublattice becomes less vacant and the chemical composition of fcc single-phase ternaries can be described as $Mo_{1-x}Cr_xN_{0.5(1+x)}$. These coatings exhibit an excellent agreement between experimentally and *ab initio* obtained lattice parameters of fcc $Mo_{1-x}Cr_xN_{0.5(1+x)}$. When increasing the N_2-to-total pressure ratio to $p_{N2}/p_T = 0.69$, the N-sublattice is already fully occupied for Cr-additions of $x \geq 0.4$, as suggested by elastic recoil detection analysis and lattice parameter variations. The latter follows the *ab initio* obtained lattice parameters along the quasi-binary MoN-CrN tie line for $x \geq 0.5$. The single-phase fcc coating with Cr/(Mo+Cr) of x ~0.2, prepared with $p_{N2}/p_T = 0.32$, exhibits the highest hardness of ~34 GPa among all coatings studied.

O–ST 08

***Ab initio* study on stacking faults in γ-TiAl**

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TiAl-based alloys have proven to be not only academically exciting, but also an industrially relevant material class. Most of them are based on a γ-TiAl, a distorted fcc-like structure. Since stacking faults (SFs) are particularly important components governing the plastic deformation in fcc-based materials, we aim on revisiting this topic using first principles calculations. Not only the SFE arepredicted and compared with literature data for different configurations (e.g., intrinsic SF, complex SF, anti-phase boundary), but the whole γ-surface (generalised stacking SF energy) is calculated using Density Functional Theory. It is demonstrated, that the superlattice instrinsic SF is energetically most favourable, followed by the complex SF and the anti-phase boundary. The last, however, is shown to be an unstable defect at 0K. These predictions are critically compared with available experimental data and classical molecular dynamics simulations, revealing severe discrepancies. Finally, a simple model is implemented to estimate alloying trends. Generally, the alloying of a ternary addition tends to decrease the SF energy.

O–MI 01

Growth of stoichiometric intermetallic phases as single phase in a temperature gradient
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Stoichiometric intermetallic phases are not straightforward to produce as single phase, especially if they melt incongruently. With a method combining mushy zone resolidification in a temperature gradient and directional solidification bulk intermetallic phases are produced in quantities of several grams [1]. Conditions close to Scheil conditions (complete mixing in the liquid, negligible diffusion in the solid) are generated by electromagnetic stirring and large sample dimensions. The solidifying phases grow spatially separated and in the sequence given by the equilibrium phase diagram for the specific composition. For obtaining an intermetallic phase directly from the melt, an overall composition that differs from that of the desired intermetallic phase is chosen. A two-phase equilibrium between liquid and the intermetallic phase is identified on the basis of thermodynamic calculations. Directional growth over extended distances is adjusted. The single phase materials are suitable for detailed characterization with respect to crystal structure, thermal properties and melting enthalpies. The method is useful for obtaining thermochemical, thermophysical and kinetic data in multicomponent systems.

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O–MI 02

The effects of thermo-mechanical treatments on the microstructure and mechanical properties of AFA steels
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In order to achieve energy conversion efficiencies of >50% for steam turbines/boilers in power generation systems, materials are required that are both strong and corrosion-resistant at temperatures greater than 973K, and are economically viable. Austenitic steels strengthened with Laves phase, B2 NiAl and $L1_2$ $Ni_3(Al,Ti)$ intermetallic precipitates, and alloyed with aluminum to improve oxidation resistance, are potential candidate materials for these applications.

The microstructure and microchemistry of a recently developed alumina-forming austenitic (AFA) stainless steel Fe-14Cr-32Ni-3Nb-3Al-2Ti (in wt.%) have been characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Two series of thermo-mechanical treatments were performed on these steels to improve their mechanical performance. During the treatments, materials were cold rolled to a 90% thickness reduction and then annealed at 1073K for different time. These thermo-mechanical treatments reduced the grain sizes to the nanoscale (~100 nm) and enhanced the room temperature yield strength to >1000 MPa.
The microstructure and microchemistry of these thermo-mechanically treated AFA stainless steels were characterized and analyzed using SEM and TEM. It was found that a solutionizing anneal at 1473K before cold rolling is effective for uniformly redistributing the large Laves phase precipitates that formed upon casting. Thermo-mechanical treatments can produce a finer-scale and more uniform distribution of both Fe_2Nb Laves phase and B2 NiAl precipitates, both in the f.c.c. matrix and at the grain boundaries. Synchrotron X-ray diffraction showed that the lattice misfit between the $Ni_3Al(Ti)$ precipitates and the iron-based f.c.c. matrix was less than 0.28% after different thermo-mechanical treatments. Both the nanoscale grains (grain boundary strengthening) and the high volume fraction of the $L1_2$ $Ni_3(Al,Ti)$ precipitates (precipi-

tate strengthening) contribute to the high yield strength, which can be up to 1289 MPa for the thermo-mechanically treated alloys.

The yield strengths of the thermo-mechanically treated AFA steels are slightly lower than that of the as-received alloy during high temperature tensile testing. Strain rate jump tests were also performed at different temperatures, the results show that the yield strength of the thermo-mechanically treated AFA steels are more sensitive to strain rate. The strengthening at high temperature mainly arises from the $L1_2$ $Ni_3(Al,Ti)$ precipitates. Dislocations and stacking faults were also observed in the Laves phase after low strain rate tensile testing at 700 °C.
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O–MI 03

NMR as a local probe for intermetallics
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Intermetallic compounds have a great impact on our daily life as they are used to build, for example, cars or bicycles and even much more simple tools like a cooking pot. Unfortunately, we have almost no idea about the origin of the fascinating properties of these materials. However, the chemical bonding should be one important parameter.

In addition, it is well known that materials' properties are highly influenced by varying local arrangements of the atoms, e.g. disorder. Assuming the crystal structure is a further key to understand the reason of the challenging properties, methods and strategies are required to study the atomic arrangements in detail.

Nuclear Magnetic Resonance (NMR) spectroscopy may serve as an ideal tool to study local ordering of the atoms, since it operates as a local probe. Diffraction methods provide information about long range atomic order. Thus, a combination of both techniques can be used to set up a structure model. With the help of Density Functional Theory (DFT) the NMR signals can be calculated by *ab-initio* methods to validate the structure model.

An additional advantage of NMR spectroscopy is the large sensitivity towards chemical bonding. The gallides of the alkaline earth metals were chosen as a model system to derive reliable NMR spectroscopic parameters for the investigation of intermetallic compounds [1-2]. The electric field gradient (EFG) turned out to be the desired quantity. It can be split into the individual contributions of the electrons according to the calculation scheme used by the program WIEN2k [3]. A systematic variation of the occupation of p_x, p_y, p_z-like electrons is observed for the above mentioned gallides [1-2].

The NMR experiments can be performed on various types of samples such as single crystals or powders with random and/or preferred orientation of the crystallites.

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O–MI 04

Intermetallic precipitates in cobalt-free, low alloyed secondary hardening steels

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Cobalt-free, low alloyed secondary hardening steels have been developed, employing combined precipitation of carbides and intermetallic particles. Current tool steel grades, which contain different types of strengthening phases, comprise high contents of expensive and scarce alloying elements to reach a certain strength level. Utilizing the beneficial effects of intermetallic phases, the addition of carbide forming elements could be reduced. To meet the required properties of high strength even at elevated service temperatures, appropriate nickel and aluminum contents are alloyed in order to precipitate NiAl-rich particles, enhancing the secondary hardening effect. Isothermal tempering experiments show the influence of alloying content on aging behavior. Transmission electron microscopy (TEM) and small angle neutron scattering (SANS) investigations reveal the influence of different heat treatment conditions on mechanical properties and contribute to establish microstructure-property correlations.

O–MI 05

Diffusion in binary silicides of iron and molybdenum

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Studies of tracer diffusion in silicides of iron and molybdenum mainly from our laboratory are reviewed. For three compositions of the DO_3-structured *Fe_3Si* tracer diffusion data of Fe and Ge are available. Fe diffusion is relatively fast and increases with Si content. Ge diffusion, which mimics Si self-diffusion, is fairly slow and almost independent of composition. A Mössbauer study of Fe diffusion revealed nearest-neighbour jumps. Positron annihilation and high pressure diffusion data indicate that, in addition to isolated vacancies, vacancy pairs also contribute to Fe diffusion. Ge and Si diffusion is presumably restricted to the Si sublattice. Tracer diffusion of Fe and Ge has been studied for B20-structured *FeSi* with the conventional tracer technique. Tracer diffusion studies after implantation of ^{31}Si (half-life 2.6 hours),
performed at the IGISOL facility in Jyväskylä, Finland, show that Ge and Si diffusion have similar diffusivities. Fe diffusion rates are considerably slower than those of Si and Ge. Tracer data of Mo, Ge and Si diffusion are available for both principal directions of the tetragonal $C11_b$-structured *molybdenum disilicide ($MoSi_2$).* For all three kinds of atoms diffusion perpendicular to the tetragonal axis is faster than parallel to it. Mo diffusion in both principal directions is by orders of magnitude slower than Si and Ge diffusion. The huge asymmetry between Mo and Si or Ge suggests that diffusion of both constituents is restricted to the own sublattice. Positron annihilation studies show formation of thermal vacancies on the Si sublattice. This suggests that Si and Ge diffusion proceed by a vacancy mechanism in the Si sublattice of $MoSi_2$. The anisotropy ratio of Si self-diffusion is attributed to a high mobility of vacancies in the Si double layers perpendicular to the tetragonal axis.

O–MI 06

Twin microstructure in 10M Ni-Mn-Ga martensite

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Ni-Mn-Ga alloys close to the stoichiometric composition Ni_2MnGa exhibit an effect known as magnetic field-induced strain (MFIS) [1,2]. This effect results from the reorientation of martensitic twin related variants involving an easy twin boundary motion.

All possible twin variants in 10M Ni–Mn–Ga alloys can be distinguished by electron backscatter diffraction. It will be shown that the twin structure in trained 10M Ni–Mn–Ga single crystals may contain three kinds of twins: main twin boundary of type I and type II, modulation boundary and a/b boundary. These twin boundaries will be characterized in great detail with regard to crystallography and morphology.

Modulation and a/b boundaries may cause an additional barrier for the motion of the main twin boundary producing MFIS.

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P–01

The influence of barrier layers (SiO_2, Al_2O_3, W) on the phase formation of RuAl thin films on LGS and CTGS substrates for surface acoustic wave technology

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The very high melting temperature of RuAl of about 2200 K, its high temperature strength as well as a strong creep and oxidation resistance result in a large potential of this material for high temperature applications, as e.g. in sensors based on the surface acoustic wave principle and the piezoelectric LGS ($La_3Ga_5SiO_{14}$) and CTGS ($Ca_3TaGa_3Si_2O_{14}$) substrates.

Pre-investigations showed a strong oxidation of the RuAl especially on LGS substrates but also on CTGS [1], so that several barrier layers have been included between film and substrate. SiO_2, Al_2O_3 as well as W thin barrier layers have been deposited with a thickness of 10 or 100 nm on which RuAl thin films with a thickness of 110 nm have been cosputtered.

A heat treatment was performed at 800°C under high vacuum conditions. Phase formation was analyzed by X-ray diffraction and surface morphology was investigated by scanning electron and atomic force microscopy. The chemical composition was determined by Auger electron spectroscopy measurements and transmission electron microscopy as well as energy dispersive X-ray analysis.

The measurements reveal a strong dependence of the RuAl phase formation and decomposition as well on the applied barrier layer material. In contrast to the films directly deposited on LGS or CTGS, the application of a suited barrier layer prevents a reaction of the RuAl metallization with the substrate and therefore improves the stability of the RuAl phase towards higher temperatures.

[1] M. Seifert, S.B. Menzel, G.K. Rane, M. Hoffmann and T. Gemming *submitted to MRX*

P–02

A new method to study the composition dependence of mechanical properties of Laves phases

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Transition-metal-based Laves phases show excellent strength properties up to high temperatures, but their brittleness at low temperature is a great drawback. Our knowledge about the plasticity of Laves phases and the way mechanical deformation proceeds is quite incomplete. The problem becomes even more complex as the existing literature indicates their mechanical properties strongly depend on composition.

A severe challenge for a systematic study of the mechanical behavior of Laves phases is the preparation of appropriate samples. Their distinct brittleness makes it difficult to prepare flaw-less bulk samples for mechanical tests. Moreover, grain size, second phases and impurities influence the mechanical behavior of bulk samples, which may mask the composition and crystal structure dependence of their mechanical properties. Therefore, we propose a new method of sample synthesis. With the diffusion couple technique, we can grow diffusion layers of target intermetallic phases covering the whole homogeneity range with dozens or even hundreds of µm thicknesses and coarse grains.

The idea is to get a series of micro-sized, single-phase and single-crystalline samples with the same orientation and different compositions using focused ion beam (FIB) cutting and to study their mechanical properties with nanomechanical testing.

Three polytypes of Laves phases exist as stable phases in the Co-Nb system, which makes this system a perfect example for a detailed study of the properties of Laves phases. In the present work, we prepared several diffusion couples to get diffusion layers of C36, C15 and C14 $NbCo_2$ Laves phases with composition gradient. The composition dependence of nanohardness was measured by nanoindentation in the layers. Single-phase and single-crystalline micropillars of Laves phases were cut along the composition gradient by FIB with the aim to study the deformation behavior and fracture toughness of the C36, C15 and C14 $NbCo_2$ Laves phases by micropillar compression and pillar splitting tests.

P–03

Phase transformation of thermal co-evaporated TiAl thin films on LGS and CTGS

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Intermetallic Ti-Al materials are already applied very successfully for components which operate at high temperatures or high mechanical load. Especially the TiAl and Ti_3Al phase have a potential to be applied as thin film electrode material for power and thermally loaded SAW (surface acoustic wave) devices. The SAW structures are preferable prepared by the lift-off process, thus the films are often deposited by a line of sight deposition technique e.g. e-beam. The results of this work form a technology basis for realization of high temperature electrode materials on high temperature stable piezoelectric substrates.

In the present paper we studied two component Ti-Al thin films on high temperature stable piezoelectric substrates, in particular the phase formation and the mechanical and electrical properties of the thin films on LGS ($La_3Ga_5SiO_{14}$) and CTGS ($Ca_3TaGa_3Si_2O_{14}$) as well as on (100)Si (reference). For this purpose Ti-Al films were co-evaporated at room temperature using an e-beam evaporator for titanium and a resistance evaporator with a boron nitride liner for the aluminum at a pressure of approx. $5x10^{-6}$ mbar. The samples were rotated and the deposition rates of both elements were controlled by an oscillating crystal measuring setup. The ratio of both elements within the samples was analyzed by inductive coupled plasma optical emission spectroscopy and the phase composition of the films was analyzed by X-ray diffraction after the samples were gradually heated up to 800°C. In addition the surface morphology of the films was investigated by atomic force microscopy and scanning electron microscopy and the electrical resistivity was measured by a 4-point probe method.

Ti_xAl films are successfully deposited in a wide composition range from $Ti_{73}Al_{27}$ to $Ti_{50}Al_{50}$. The measurements reveal a strong dependence of the Ti-Al phase formation and decomposition on temperature and used substrate material. The potential of TiAl and Ti_3Al films as SAW electrode material is discussed.

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P–04

Compression of micropillars of single crystalline Mo_5SiB_2

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Mo_5SiB_2 with the tetragonal $D8_l$ structure is one of the promising refractory silicides for ultra-high temperature structural applications because of its very high melting point (2200°C), good oxidation resistance and excellent high-temperature strength. Previous researches on the deformation behavior using single crystalline Mo_5SiB_2 and multiphase Mo-Si-B alloys have revealed the activation of dislocations with Burgers vectors of <100>, <110> and [001] at high temperatures above 1200°C. However, the details of the operative deformation modes in Mo_5SiB_2 phase have not been fully clarified yet. Recently, micropillar compression tests of single crystalline materials have been found to be useful for studying deformation behavior of brittle materials such as Si, GaAs at temperatures far below their ductile to brittle transition temperatures observed for bulk-scale specimens. In the present study, the micropillar compression tests were applied to Mo_5SiB_2 single crystals in order to investigate their deformation behavior at room temperature. Micropillars of single crystalline Mo_5SiB_2 with rectangular cross sections were prepared by focused ion beam technique and tested in compression at room temperature as a function of the loading axis orientation and the specimen dimensions. Plastic deformation was confirmed for the [021]- and [100]-oriented micropillars with side lengths below 10 micron. Yield stress values were extremely high about 6 GPa and exhibit the size-scale effect, i.e., 'smaller is stronger' phenomena, following power-law relationships.

P–05

Atomic scale analyses of deformation modes in Mg-TM-RE LPSO phases by STEM

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New light-weight structural alloys developed in the Mg-TM (transition-metal)-RE (rare-earth) based systems have attracted considerable attention because of their high strength and good ductility. Their excellent mechanical properties have been considered to be related closely to the deformation behavior of the platelet precipitates with long period stacking ordered (LPSO) structures, which are characterized by the periodic stacking faults associated with the enrichment of TM and RE atoms in four consecutive atomic layers within the hcp stacking of parent Mg. However, the deformation mechanisms of the LPSO phases are still unsolved, mostly because the lack of the information on the crystal structures. Recently, we have successfully determined the crystal structures of the LPSO phases by atomic resolution scanning transmission electron microscopy (STEM) and transmission electron microscopy (TEM). In the present study, defect structures in the Mg-TM-RE LPSO phases introduced by room temperature compression tests were investigated by atomic-resolution STEM and TEM. The Mg-Al-Gd ternary alloy containing the Mg-Al-Gd LPSO platelet precipitates with the 18R-type stacking sequence in the Mg-matrix is confirmed to be deformed by the *c*-axis tension twinning on {11-21}, whose passage causes bending of the LPSO platelets. The bending of the LPSO platelets is confirmed to be caused by the deformation twinning equivalent to the {11-21} twinning in the Mg matrix. The deformation twin in the LPSO phase is frequently accompanied by the accommodation kink, which is composed of regularly spaced edge dislocations with the Burgers vector parallel to [11-20]. Atomic arrangement at the twin boundary regions and around edge dislocations in the Mg-Al-Gd and Mg-Zn-Y LPSO phases investigated by the ultra-high resolution STEM will be presented.

P–06

Phase field simulation of Al_2Mg_3 and $Al_{12}Mg_{17}$ intermetallic compound formation in FSpW of AA5754 alloy to AZ31 alloy

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In friction spot welding (FSpW) of AA5754 alloy to AZ31 alloy, Al_2Mg_3 and $Al_{12}Mg_{17}$ intermetallic compound (IMCs) have detrimental effect on lap shear strength of welded joint. It is almost impossible to understand such IMCs formation kinetics dynamically and quantitatively by experiments. In this paper, a mathematical and physical based multi-phase field model is developed to simulate Al_2Mg_3 and $Al_{12}Mg_{17}$ formation between interface of aluminum and magnesium sheets under virtual FSpW conditions, that is, couples of temperature, strain rate and strain and accumulated plastic deformation energy boundary conditions are defined in phase field calculation domain. The boundary condition dependent diffusion coefficient and interface mobility are considered for calculation. Gibbs energies of different phases are described using Thermo-Calc and Panengine software. IMC formation and growth in Al and Mg interface, as well as grain growth of IMC are simulated in the established framework. IMC growth kinetics is analyzed in terms of IMC thickness and Al_2Mg_3 and $Al_{12}Mg_{17}$ grain numbers. IMC grows very fast due to enhanced diffusion and interface mobility under the three conditions above. Collaboration of fine IMCs grains can retard further IMC growth into Al and Mg matrix. The predicted IMCs morphology and final thickness at certain conditions is comparable with experimental results.

P–07

Room temperature deformation behavior of hard intermetallics and ceramics investigated by micropillar compression tests

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Hard intermetallic compounds and ceramics have been widely used as strengthening phases in various metallic and intermetallic alloys mostly because of their extremely high strength. Since most of these hard materials possess very complex crystal structures, they generally have a limited number of operative deformation modes, which results in their brittleness especially at low temperatures. Although they exhibit brittle nature in bulk-scale mechanical tests, the dislocation activation has been known to be possible by indentation tests and uniaxial compression tests under a hydrostatic confining pressure. However, it is difficult to interpret the results obtained by these mechanical tests since the stress states are complicated. Very recently, the micropillar compression test has been introduced as a new promising method for investigating the mechanical behavior of brittle materials such as semiconductors, ceramics and intermetallics with complex crystal structures at low temperatures far below their brittle to ductile transition temperatures observed in bulk-scale mechanical tests. In the present study, we have applied the micropillar compression tests systematically to some complex intermetallic compounds such as transition metal silicides and Laves phases as well as some ceramics (6*H*-SiC, B_4C) in order to elucidate deformation mechanisms of these hard materials at room temperature. Single-crystalline micropillars of various hard materials with rectangular cross sections were prepared by focused ion beam technique. Micropillar compression tests were conducted at room temperature as a function of the loading axis orientation and specimen size using a nanoindenter equipped with a diamond flat punch. Plastic deformation is observed for some of the hard materials tested. Yield stress values generally increase with the decrease in the side length following a power-law relationship. Possible mechanism for the size-scale effects will be discussed based on the single-arm dislocation source model.

P–08

Micropillar compression of single crystals of $L1_2$-$Co_3(Al,W)$

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Recently, a new ternary $L1_2$ (γ') phase $Co_3(Al,W)$, which can coexist with a fcc solid-solution phase (γ) based on Co, has been discovered. We investigated the compression deformation behavior in polycrystals of $L1_2$-$Co_3(Al,W)$ and found that $Co_3(Al,W)$ exhibits a positive yield stress-temperature dependence as in the case of Ni_3Al and many other $L1_2$ compounds although its temperature region is quite narrow (950-1100 K). Due to the difficulties in growing large single crystals, however, the critical resolved shear stress (CRSS) of $L1_2$-$Co_3(Al,W)$ has never been measured. Recent years, fabrication processes with precise control of material dimensions down to the nanometer level, for example, with the focused ion beam (FIB) method, has been developed so that it becomes possible to investigate mechanical properties at these small scales. Employing this method, even from polycrystals, the CRSS value can be obtained through compression tests of single crystal micropillars with different sizes. In the present study, we investigated the compression deformation behavior of single crystal micropillars of $L1_2$-$Co_3(Al,W)$ in order to elucidate its CRSS value at the bulk scale. Single crystal micropillars with dimensions from approximately 1x1x3 to 10x10x30 μm were cut out from a polycrystal ingot with a nominal composition of Co-12Al-11W (at.%). The crystal orientations of the micropillars were determined by EBSD. Two loading axes with similar Schmid factors for (111)<-101> slip but different N-factors, the ratio between the Schmid factors for (111)<-101> and (010)<-101> slips, were selected to investigate the orientation dependence of CRSS in $L1_2$-$Co_3(Al,W)$. The CRSS value of the micropillars shows an inverse power-law scaling against the specimen size as in the case of pure fcc and bcc metals. The bulk CRSS value is estimated by extrapolating the power-law scaling to the range of 20-30μm in pillar size and compared with that of $Ni_3(Al,W)$.

P–09

Precipitation behavior of Co_7Nb_2 from supersaturated Co solid solution in the Co-Nb binary system

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Some intermetallic compounds precipitated by peritectoid reaction show extremely slow reaction rate in spite of their high reaction temperature. To elucidate fundamentals of this kind of phenomenon is important for alloy development with utilizing these intermetallic compounds. Co_7Nb_2 forms in the manner of peritectoid reaction at high temperature (1359K), and it shows some curious properties. One of the authors revealed that the reaction rate of Co_7Nb_2 was extremely slow in both formation and decomposition [1], and that Co_7Nb_2 can be strongly deformed at room temperature by hammering without fracture [2]. However, the detailed mechanisms of them are still unclear. In the present study, authors have prepared the Co-1Nb, 2Nb and 4Nb (at%) binary alloys in order to elucidate the precipitation behavior of Co_7Nb_2 from simply supersaturated Co solid solution. Pure Co and the Co-22.2Nb binary alloy have been also prepared for the comparison. Various thermal analyses by differential scanning
calorimeter were carried out for the samples after homogenization heat treatment at 1513K for 10h. Crystal structure was investigated by X-ray diffraction and electron backscatter diffraction. Microstructural observations were also performed by optical and scanning electron microscopies. It is clarified that Co_7Nb_2 is precipitated from supersaturated Co solid solution in the manner of discontinuous precipitation, and its reaction rate is rather fast. The crystal structures of Co solid solution before and after discontinuous

precipitation of Co_7Nb_2 are identified as fcc and hcp, respectively. It implies that Nb in Co solid solution stabilizes fcc structure, and it could be intimately related to the precipitation behavior of Co_7Nb_2.

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P–10

Primary phase fields of complex metallic alloy phases in the Al-Mg-Zn System close to the Mg-Zn subsystem

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Complex metallic alloy phases (CMA´s) are a fascinating class of materials. They comprise intermetallic compounds with giant unit cells and quasicrystalline phases. Four complex metallic alloy phases, called τ_1 [1], τ_2, q [2], and Φ [3] have been reported as ternary compounds in the Al-Mg-Zn system. The q phase is quasicrystalline, τ_1 and τ_2 Bergman cluster approximants and Φ a decagonal approximant. Recently, we have reported the crystal structures and the homogeneity ranges of Φ [3] and τ_2 [4]. During this investigation a number of new CMA´s close to the Mg-Zn subsystem have been observed. λ and the τ_d form at the composition $Al_3Mg_{41}Zn_{56}$ with 1488 atoms and 308 atoms per unit cell as low and high temperature phase, respectively and the β_{Zn} phase with 1168 atoms per unit cell at the composition $Al_8Mg_{43}Zn_{49}$. We report on the determination of the primary phase fields and the type of four phase reactions for the new phases by microstructural and DSC investigations of more than 80 alloys close to the Mg-Zn subsystem.

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P–11

Microstructural investigation of the intermetallic composites NiAl-(34-x)Cr-xMo before and after creep

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Structural materials for energy efficient applications have been developed for many decades. The intermetallic compound NiAl possesses promising properties for high-temperature applications. It combines a low density (5.7 g/cm³), a high melting point (T_m = 1638°C) with a good corrosion as well as oxidation resistance. Unfortunately, the creep resistance decreases dramatically beyond 600°C, partly because of the relatively open B2-ordered crystal structure. Refractory elements, i.e. Chromium, Molybdenum and Rhenium can strengthen the intermetallic NiAl by forming a second fibrous or lamellar phase during directional solidification (DS). Due to DS, the reinforcing phase has a distinct relation to the NiAl matrix which is parallel to the solidification direction, e.g. in the case of NiAl-34Cr and NiAl-31Cr-3Mo the orientations are [100] and [111], respectively.

This study represents the microstructural analysis of NiAl-(34-x)Cr-xMo composites before and after creep. Therefore creep tests under constant compressive stresses (100 MPa–300 MPa) and at constant temperatures (900°C–1100°C) are performed showing a significant creep rate minimum at low true strains. TEM investigations on as-DS NiAl-34Cr reveal in longitudinal section dislocation networks in the Cr-fibers with Burgers vectors of and an average dislocation distance of around 96 nm. These interface dislocations reduce the coherency stresses which are caused by the lattice mismatch of the two phases (0.24% for NiAl-34Cr determined by X-ray measurements). Dislocations from the NiAl matrix can pass the interface leaving incomplete dislocations which hinder further dislocation motion (see also [1] and [2]. The analysis will compare work done for (fibrous) NiAl-33.5Cr-0.5Mo and (lamellar) NiAl-31Cr-3Mo.

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P–12

The massive transformation in a quaternary Ti-Al-Nb-Ta alloy

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The fact that TiAl alloys only have limited room temperature ductility makes alloy and microstructural optimisation indispensable. One way to improve the properties is to generate an alternative microstructure, by utilizing the cooling-rate dependent massive transformation and subsequent annealing treatments. Such a microstructure is known as a “convoluted microstructure”. During slow cooling from the single high-temperature phase field of hexagonal α-Ti(Al) (hcp structure) phase, lamellae of the tetragonal γ-TiAl phase ($L1_0$ structure) precipitate on α-basal planes according to the orientation relationship: {111} γ || (0001) α and <1-10> γ || <11-20> α. Faster cooling can result in a massive transformation of α-Ti(Al) to γ-TiAl. During subsequent annealing, α_2 lamellae precipitate on the tetrahedral planes (111) of the γ phase resulting in the aforementioned “convoluted microstructure”.

In this study a Ti-45Al-4Nb-4Ta (at.%) alloy was investigated using *in situ* high-energy synchrotron X-ray diffraction. *In situ* experiments enable continuous monitoring of phase evolution during heating and cooling. In particular the transformation start temperature, the critical cooling rate, and the undercooling required for the massive transformation, as well as for subsequent α_2 precipitation during annealing have been investigated. The microstructure developed after the massive transformation and after subsequent annealing has been characterised by EBSD.

P–13

Determination of the crictical resolved shear stress in a NiAl-Cr composite by discrete dislocation dynamics

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Within the research program IMD www.imd.kit.- edu) a new high temperature superalloy shall be developed. The microstructure consists of a NiAl matrix [1], which alone has poor mechanical properties at high temperatures, and Cr fibers, which block the motion of dislocations within the NiAl matrix and increase the creep resistance significantly. The microstructure is obtained by solidification at the eutectic composition for the ternary system and under ideal conditions long Cr fibers are expected [2, 3]. In a two dimensional Cross-section with the normal parallel to the Cr fibers axis a close to hexagonal arrangement of the fibers cross-sections is observed. In order to determine the Critical Resolved Shear Stress (CRSS) for a dislocation passing through this almost hexagonally arranged obstacle field discrete dislocation dynamics (DDD) simulations are performed [2, 5]. The role of the irregularities in the arrangement and the fibers diameters in the experimentally measured microstructures is explored by a systematical variation of the obstacle distribution in the simulations. The simulations use periodic boundary conditions to eliminate surface effects and the fibers are treated in this first step as non-shearable and those bypassing occurs by the Orowan mechanism. In order to determine the CRSS valid for this superalloy the length L between two centers of Cr fibers is varied. Furthermore several distributions of the Cr precipitates taking in consideration the variation of the length L and Diameter D of the fibers are produced on the basis of the experimental received data and used in the simulation set up [4]. It is observed that, with increasing irregularity the CRSS as their spread in the obtained increases. Furthermore the effect of the elastic interaction between multiple dislocations on parallel planes gliding through this obstacle field shall be addressed. At the end the softening effect at the boundary interface between Cr fibers and NiAl matrix doing to lattice mismatch is investigated and it was found that the CRSS decrease in this case for non shearable fibers of about 20%.

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P–14

Atom probe study of ω_o-phase in a β-phase containing TiAl alloy

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Advanced multi-phase γ-TiAl based alloys are envisaged as materials for high-temperature light-weight structural components in modern aero and automobile engines. Their material properties, e.g. ductility, are highly dependent on the morphology of the constituent phases. Especially in the case of β-solidifying alloys such as the so-called TNM alloy, which are gaining considerable attention, a volume fraction of the β_o-phase is retained to RT. In order to achieve a β-solidification pathway alloying with β-stabilizing elements, e.g. Nb and Mo, is conducted. However, these alloying additions not solely change the transformation pathway, but also result in the introduction of additional phases, e.g. the ω_o-phase, which is of significant importance as it can lead to hardening of the material.

Aim of this study was the investigation of ω_o-particles in the TNM alloy present after creep testing. These particles were observed to be embedded in the β_o-phase. Microstructural characterization was conducted using transmission electron microscopy (TEM), transmission electron backscatter diffraction (t-EBSD) and atom probe tomography (APT). Evaluation of APT data yielded the chemical composition of the ω_o-precipitates and the surrounding β_o-phase. The ω_o-phase was observed to reject Mo, resulting in an enrichment of the β_o-matrix. Moreover, proximity histograms of the interfaces were derived showing segregation of Mo in the vicinity of the interface. These accumulations were addressed by calculation of the interfacial excess. Furthermore, the interfacial width was determined by evaluation of the concentration profile as proposed in [1].

Gained data significantly contribute to the understanding of evolution of the ω_o-phase in advanced β-solidifying TiAl alloys under creep conditions.

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P–15

Microstructure and phase constitution of intermetallic layers fabricated by selective laser melting of elemental Al and Ti powders

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The investigation of intermetallic layers fabricated by selective laser melting (SLM) of equimolar mixtures of Al and Ti elemental powders was carried out to understand a correlation of microstructure, homogeneity and phase constitution with laser processing parameters. The SLM was done using fiber laser with 1075nm wavelength with a focal spot of 80μm, and 150W laser power. The specimens were produced with 1.2m/s laser speeds, using one-pass and two-pass scanning strategies. Obtained layers were characterized by means of LEO 1350 FEG-SEM equipped with Oxford Instruments INCAx-sight EDX detector. The Seifert 3000 PTS X-ray diffractometer with $Cu_{K\alpha}$ radiation was used for phase analysis. The results show challenges in manufacturing of homogeneous intermetallic material by means of SLM. The results revealed deviations in chemical composition of tracks compared to nominal mixture, phase constitution was also found different from equilibrium. The findings are discussed in relation to incomplete remixing of elements in the molten pool, possible evaporation of elements due to local melt overheating and rapid cooling preventing ordering processes. Opportunities to improve quality of intermetallic materials manufactured by SLM discussed in terms of optimization of laser power and scanning speed, initial powder composition and post heat treatment.

P–16

$Ga_{1-x}Sn_xPd_2$ ($0 \le x \le 1$) as catalytic material for the semi-hydrogenation of acetylene

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$GaPd_2$ is known to be a highly selective and stable catalyst for the semi-hydrogenation of acetylene [1]. A continuous solubility between the isostructural $GaPd_2$ and $SnPd_2$ compounds (Co_2Si-type structure, *Pnma*, *oP*12) was revealed during systematic investigation of the ternary Ga-Sn-Pd system. The samples were synthesized from the elements by arc melting, annealed in alumina crucibles placed in evacuated silica tubes and subsequently quenched in water. Phase characterisation was conducted by means of powder X-ray diffraction analysis (PXRD) and scanning electron microscopy with energy dispersive X-ray spectroscopy (EDXS). Powdered samples with the nominal composition $Ga_{33.3-x}Sn_xPd_{66.7}$ (x = 0, 5.3, 9.3, 13.3, 15.3, 17.3, 19.3, 21.3, 28.3, 33.3) were tested in this catalytic reaction.

According to measurements, the catalytic properties are strongly influenced by chemical composition and thus the electronic structure while there is no change of the geometric structure over the whole concentration range.

All tested samples show high selectivity to ethylene on a comparable level of conversion. The activity increases by reducing the amount of tin in the sample. The maximum of activity was detected at 9.3 at. % Sn. Samples with even less Sn content showed reduced activity.

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P–17

The C15 Laves phase in system U-Zr-Mo

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Metallic uranium is the ideal material for nuclear fuels. It presents the highest density of uranium atoms among all other concurrent materials, allowing for the operation of the reactor under lower enrichment levels, and present other advantages like optimal heat conductivity and the ability to accommodate stresses by plastic deformation. Pure uranium, however, shows a base centered orthorhombic structure in the reactor's operation temperature. This allotrope shows high mechanical and thermal anisotropy, which could lead to severe failures in service. To solve this problem the addition of molybdenum, zirconium and other alloying elements have been sugested to stabilize the high temperature body centered cubic phase (which is isotropic). From the literature it is known that system Zr - Mo possess an intermetallic $MoZr_2$ Laves phase (C15), so, at least this intermetallic is predicted to exist in the ternary system. Three U-Mo-Zr alloys were arc melted under argon atmosphere, with nominal compositions U - 9wt% Mo - 3 wt% Zr, U - 6 wt% Mo - 6 wt% Zr and U - 3 wt% Mo - 9 wt% Zr. The samples were characterized by scanning electron microscopy and EDS mapping. The as cast alloys present only almost pure zirconium precipitates, but the heat treated alloys presents free Zr in dendritic morphology and $MoZr_2$ in spherical morphology.The size and distribuition of $MoZr_2$ precipitates was characterized in function of Zr/Mo ratio, leading more intense precipitation, but with smaller particles, as this ratio decreases. The solubility of uranium in the precipitates was measured and found to be negligible.

P–18

The effects of annealing on the microstructure and mechanical properties of f.c.c./B2 $Fe_{28}Ni_{18}Mn_{33}Al_{21}$

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As-cast $Fe_{28}Ni_{18}Mn_{33}Al_{21}$, which consists of aligned, 50 nm, (Ni, Al)-rich B2 and (Fe, Mn)-rich f.c.c. phases, was annealed at a variety of temperatures up to 1423 K for up to 250 h and the microstructures and mechanical properties were examined. It was shown that the as-cast microstructure arises from a eutectoid transformation at ~1300 K. Annealing at temperatures ≤1073 K produces β-Mn-structured precipitates, while annealing at temperatures >1073 K leads to dramatic coarsening of the two-phase B2/f.c.c. microstructure, but does not produce β-Mn precipitation. Interestingly, annealing at temperatures >1073 K delays the onset of β-Mn precipitation during subsequent anneals at lower temperatures. Coarsening the B2/f.c.c. lamellar structure by annealing at higher temperatures softens it and leads to increases in ductility, from fracture before yield to ~ 8% elongation: the presence of β-Mn precipitates makes the fine, brittle B2/f.c.c. microstructures even more brittle, but significant ductility is possible even with β-Mn precipitates present if the B2/f.c.c. matrix is coarse and more ductile.

Annealing at 1173 K for a variety of times up to 250 h was used to produce a wide range of phase widths (50 nm - 2.5 μm) over which to quantify the effects of changing the phase width, l, on the mechanical properties. The coarsening kinetics over this two orders of magnitude change could be described by $R^2 - R_o^2 = kt$, where R is the average of the B2 + f.c.c. phase width after time *t* at 1173 K, R_o is initial phase width, and k is a constant. It was found that the yield strength, s_y, follows a Hall-Petch-type relationship, i.e. $s_y = s_o + k_y \lambda^{-1/2}$, where s_o is the strength for the single-phase material, and k_y is a constant. Interestingly, the work-hardening rate also followed a $\lambda^{-1/2}$ relationship, while the elongation to failure increased as l increased from failure before yielding in the as-cast material to ~7% for the material with the largest λ.
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P–19

Laser cladability of gradient multi-layers in Fe-Al intermetallic system

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The laser welding and cladding of dissimilar Fe and Al alloys are important for aerospace and automobile industries where serious difficulties are caused by high brittleness of the intermetallide phases generated in the melting pool.
The applicability of three-dimensional (3D) laser cladding for fabrication of functional gradient and building Fe_xAl_y (x, y = 1, 2, 3) intermetallic multilayer structures was studied experimentally. It was shown that the laser additive manufacturing process implementation has a tendency to form heterogeneous phases of Fe_3Al and FeAl. Microhardness growth from 300 HV to 900 HV was obtained for the same sample due to change of elements ratio in the Fe - Al system during the 3D laser cladding. It was also observed that sizes and boundaries of transition zones between the powder compositions with different components and of corresponding Fe_xAl_y intermetallic phases depend on the laser synthesis conditions and can thus be controllable. The possibility to control hardness of the multi-layer structure by changing powder com-

position and using an appropriate CAD modeling can expand the range of 3D functional graded material applicability in aerospace or nuclear industries.

P–20

Void-free interconnection through dual-phase intermetallics in solid-liquid interdiffusion bonding
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Solid-Liquid Interdiffusion Bonding (SLID) provides the advantages of low temperature bonding process and high temperature application, which has been widely used in the fabrications of high power modules, thermoelectric modules, high power LED packages and 3D-IC packages. For this bonding technique, low melting point thin film interlayer (LT) is inserted between two metallic layers with higher melting point (HT) and heated above the melting point of LT-thin film interlayer. After the interfacial reactions, the liquid LT thin film reacts completely with the HT metallic layers and transfers into solid intermetallic compounds, which possess much higher melting temperature than that of the original LT interlayer. However, the uneven growth of intermetallics front often causes the appearance of a large amount of voids, which degrade the bonding strength and electrical and thermal conductivities. An example was shown in the SLID bonding of 5µm Ni/ 3µm Sn/ 5µm Ni between two Si substrates, which resulted in the formation of many voids at the interface between Ni_3Sn_4 intermatallics layers and a shear strength of 13 MPa. An improved method through the employment of an innovative concept of dual-phase intermetallics has been proposed to diminish the voids and increase the bonding strength. This method uses an additional 2µm Ag thin film to be inserted into the 5µm Ni/ 3µm Sn/ 5µm Ni sandwich to form the 5µm Ni/ 2µm Ag / 3µm Sn/ 5µm Ni or 5µm Ni/ 1.5µm Sn/ 2µm Ag / 1.5µm Sn / 5µm Ni metal stacks. After SLID bonding, the second Ag_3Sn intermetallics fill the void of the first Ni_3Sn_4 intermatallics to achieve a void-free interconnection. The shear strength was drastically increased to 20 MPa.

P–21

Mechanical properties of a forged Fe-26Al-1.5Ta compressor blade

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Most of the interest in iron aluminide based alloys has been focused on their possible structural application as replacements for Fe-based materials and stainless steels because of different advantages, like, high corrosion resistance to oxidizing environment at relatively high temperature, low density in comparison with stainless steels, excellent wear resistance, convenient strength at elevated temperatures, and low cost of raw materials. However, their ductility at low temperatures and creep strength at high temperatures have to be improved. For improving strength at high temperatures, different approaches have been employed, like, incoherent and coherent precipitates or increasing the ordering in the matrix. For enhancing ductility thermomechanical processing such as hot forging has been tested [1, 2].

In the present work, a number of pancake samples were forged at different temperatures and with various deformation degrees, which were investigated after annealing at 700°C for different times. In a second step a number of compressor blades have been fabricated by forging, showing the feasibility to produce such parts by this technique. The microstructural evolution was characterized by light optical microscopy (LOM), scanning electron microscopy (SEM), and electron backscatter diffraction (EBSD). The compositions of individual phases were analyzed by energy- and wavelength dispersive spectrometry (EDS, WDS).
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P–22

Fundamental studies on casting of iron aluminides

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Iron aliminides are often quoted as prospective materials for technological applications at moderate to high temperatures, but contrary to nickel and titanium aluminides, they have not yet, to the best knowledge of the authors, reached the status of commercial alloy for some particular application niche. One of the most severe drawbacks, reported for iron aluminides, is the limited room temperature ductility, which impairs the use of well stabilshed processing routes for metallic alloys, like cold rolling and stamping, for example. Limited ductility, however, is not new in metallurgy. Many well stablished commercial alloys, like gray cast irons or unmodified Al-Si eutectic alloys, have negligible (or even non-existant) room temperature ductility and still are used with success in large quantities in several important technological applications. These alloy, obviously, are proccessed by casting. When it comes to iron aluminides, however, it is surprizing the lack of information about trivial casting properties, which are necessary for the development of this proccessing route. The present work deals with the measurement of the alloy solidification contraction, a critical quantity for gating and risers project for any casting part. The prospective measured methods are reviewed and applied to alloys containing 30at.% Al, with and without chromium (6at.%) and molybdenum (0.5at.%) additions.

P–23

Solidification processing of Nb silicide based alloys – alloy design and macrosegregation of alloying additions

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There is strong industrial preference for cast Nb silicide alloys. Industry looks forward to having directionally solidified (DS) and even single crystal (SX) Nb silicide based alloys. This expectation is based on familiarity with production and use of cast Ni superalloys for more than 30 years.

In the open literature the solidification processing of Nb silicide based alloys has attracted very little attention compared with their microstructures, mechanical properties and oxidation. The literature on macrosegregation in “conventional alloys” gives one an idea about the complexity of this phenomenon and how limited our understanding of macrosegregation is, even for ferrous alloys, superalloys and light metal alloys that have been studied extensively and for which there is data to support macrosegregation modelling.

The presentation will discuss clean melting and casting and directional solidification of Nb silicide based alloys with emphasis on the macrosegregation of Si. The latter will be studied using material parameters based on the melting temperatures and enthalpies of melting of sd and sp electronic configuration alloying elements in Nb silicide based alloys. Rules to help alloy designers use to their advantage macrosegregation of alloying additions will be discussed.

P–24

Combined *ab initio*, semiempirical and experimental approach

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Mn-based systems play an important role in modern materials, e.g. Mn and Ta are used in thermoelectric coolers at low temperatures and Mn-Ti alloys can be found among hydrogen-storage or high-strength materials. Hence, the thermodynamic functions describing the behaviour of phases included in both Mn-Ta and Mn-Ti systems have to be determined properly to enable consequent prediction of phase equilibria in higher-order systems. From this reason a combined *ab initio* and CALPHAD modelling was performed including the results of previous studies (Mn-Ta [1-5], Mn-Ti [6-9]). To get the information on energetics of hypothetical phases inevitable in thermodynamic modelling (end members), *ab initio* calculations based on equilibrium structure parameters were performed. This work presents the implementation of *ab initio* data to the thermodynamic assessments and phase diagram calculations of the above mentioned systems. The comparison of calculations with experimental data, especially from [1,6,8,10] is presented.

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P–25

***Ab initio* and phase-field study of the Ti-Fe eutectic system**

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Eutectic Ti-Fe composites exhibit a high strength (~1000 MPa), very good ductility, and sufficient corrosion resistance to consider them as very promising candidates for numerous aerospace and automotive applications. The dual-phase Fe-Ti eutectics contain rather brittle FeTi intermetallic phase with the B2 structure and softer and more ductile ß-Ti(Fe) alloy with varying Ti concentration (depending on the cooling rate). Motivated by the fact the ß-Ti(Fe) phase cannot be prepared as a single-phase material with varying Ti content (what hinders its experimental testing), we study the Ti-Fe alloys covering a broad range of Ti concentrations using quantum-mechanical calculations [1,2]. Employing the density functional theory, we correctly predict phases that are stable at both low and elevated temperatures in agreement with the experimental Fe-Ti phase diagram. Analyzing the electronic structure of the stable phases, we explain their thermodynamic stability as stemming from a composition-sensitive reduction of density of states at the Fermi energy. Combining the thermodynamic aspects with the study of both single-crystalline and polycrystalline elasticity of various Fe-Ti alloys, the origin of ductility and softness of the ß-Ti(Fe) phase is identified.

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P–26

Experimental investigation and thermodynamic modeling of Al-Mo-Ni System and its extension into NiAl-Cr-Mo system

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The intermetallic compound NiAl possesses attractive properties for high temperature structural applications. However, their utilization is limited due to their room temperature brittleness and reduced high temperature creep resistance. These disadvantages can be removed by manufacturing a metal-matrix composite of NiAl strengthened by embedded fibers of refractory metals such as Cr and Mo. The system NiAl-(Cr, Mo) offers the opportunity for an *in-situ* preparation of these composites by directional solidification of alloys with eutectic composition. In the present work, key experiments are carried out. Thermodynamic assessment of the system Al-Mo-Ni and its extension into NiAl-Cr-Mo system are presented in order to support the selection of alloys for directional solidification.

Assessments of the Al-Mo-Ni system are already reported in the literature but these are impaired by problems, particularly in the subsystem Al-Mo. Previous assessments either cannot properly reproduce the congruent melting point of AlMo or an artificial inverted miscibility gap is created in the liquid phase. Furthermore, in the available assessments of Al-Mo-Ni, no suitable models are applied for the ordering transition among the A2/B2 phases, which is indispensable for the merger of this system with the dataset of Al-Cr-Ni from literature. The present work provides a new optimization for Al-Mo-Ni where these drawbacks are corrected. This assessment is further merged with the dataset of Al-Cr-Ni and extended into the NiAl-Cr-Mo system. The optimization focuses on the eutectic equilibria between the liquid, NiAl (B2) and the (Cr, Mo) phase A2. First calculations with quaternary dataset are compared with the experimental results of the quaternary alloys prepared by arc melting.

P–27

Integration of thermodynamic energies in phase-field simulations – ternary solidification

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The phase-field method has become a useful and well established technique for the study of thermodynamically-driven phase transformation processes. For the modeling of the microstructure evolution of a directional solidified eutectic alloy with phase-field simulations, thermodynamic databases are an important source of information.

The necessary input functions for phase-field simulations, based on a grand-potential formalism, are the chemical and grand-potentials, which define the driving force of the microstructure evolution. These quantities are not directly provided by the CALPHAD approach.
The presented approach introduces a standardized and automated workflow of the transformation of thermodynamic databases from CALPHAD to effective usable functions in the framework of phase-field simulations. For the determination of the input parameter functions of the Gibbs energies from the databases, two different fitting methods are developed. To improve the accuracy of the functions for each involved phase, the information in a small predefined concentration range around the points of equilibrium concentration are considered. The equilibrium conditions at certain temperatures are calculated from the

database. Besides the standard approach with the method of least squares, an alternative fitting method is used. In this approach, the approximated function exactly fits the point of equilibrium concentrations for each phase as well the first and second derivate. Both approximations methods are adapted with a parabolic fitting approach. The least square method is also used for an ideal solution approach. The resulting parameter functions are applied to phase-field microstructure simulations of directional solidification in ternary eutectic alloys. Different pattern formations are presented for the systems Ag-Al-Cu, Al-Cr-Ni and Nb-Si.

P–28

Crystal structures of three Ni-Ti-Si containing silicides and their oxidation resistance in air

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Ni-Ti-Si silicides are potential protective coatings for vanadium based alloys envisaged as cladding material for sodium cooled IVth generation nuclear reactors [1]. Some of these materials have the capability to form in air a mixed oxide layer composed of silica and rutile having a high efficiency to limit oxidation. Therefore they could be of interest in other application where silica would be prefer to Al_2O_3 or Cr_2O_3 former coatings,such as those containing chloride and sulphate salts [2] for example.

For this study, three silicides with compositions Ni_4TiSi_4, $Ni_4Ti_4Si_7$ and $Ni_3Ti_3CrSi_6$ were manufactured using the powder metallurgy route.The first step for preparation consists of inductive melting of stoichiometric mixtures of pure metals and silicon (high-purity Ni, Ti, Cr and Si) in a water-cooled copper crucible. Then, the ingots were hand-crushed into a powder until a grain size of less than 80 µm was obtained. A sample of the powder was retained for X-ray characterisation. The rest was densified by uniaxial hot pressing under argon to produce dense samples.

Diffraction patterns were first used in the 'profile matching' mode of Fullprof in order to refine the cell and profile parameters knowing that Ni_4TiSi_4, $Ni_4Ti_4Si_7$ and $Ni_3Ti_3CrSi_6$ crystallised in Pnma, I4/mmm and $P4_2$/mbc space groups respectively. For Ni_4TiSi_4 and $Ni_4Ti_4Si_7$, the used models led to the expected compositions. For $Ni_3Ti_3CrSi_6$, the composition varied from that of the $Nb_3Fe_3CrSi_7$ prototype. Therefore occupation ratio of Cr containing sites was optimized. The final Rietveld refinement parameters led to satisfactory confidence factors (Rwp < 8%). The Ni_4TiSi_4 and $Ni_4Ti_4Si_7$structures consisted of atomic planes stacking along the b-axis; they can therefore be considered a pseudolamellar structure. In this work all these structures were schematically described highlighting this pseudolamellar feature.

Then the oxidation behaviour was investigated. First, it has to be noticed that the Si content of these three silicides only differed of 1 at.%. However the Si activity and peculiarly the content of some stacking planes for which amounts in Ni, Cr, Ti and Si changed from one to another silicide can significantly affect the oxidation behaviour. The study was performed at 1100°C in air by thermogravimetry. Results indicated that the $Ni_4Ti_4Si_7$ presented the lower mass gain in these experimental conditions. The full characterization of thecorrosion products formed at the top of the samples and the resulting cross sections are in progress.

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[2] Ishitsuka T, Nose K, Corros.Sci.2002;44:247

P–29

Phase Stability of FeCr-σ Phase in Fe-Cr-Ni-M Quaternary System at Elevated Temperatures
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The FeCr-σ phase with the crystal structure of $D8_b$ (*tP*30) has been regarded as a detrimental phase in austenitic heat-resistant steels and alloys, but it could be a promising strengthener of the fcc matrix phase, just like Fe_2Nb Laves phase, if the poor phase stability can be improved up to higher temperatures. In Fe-Mo and Cr-Mn binary systems, there exists high-temperature σ phase region above 1508 K and 1273 K, respectively, up to melting temperature. In the present study, thus, phase equilibria among the σ/γ/α phases in Fe-Cr-Ni ternary and Fe-Cr-Ni-M (M: Mo, Mn) quaternary systems have been investigated at elevated temperatures above 1173 K, in order to identify the effect of M addition on the σ phase stability. The alloys studied were Fe-29 Cr-20 Ni (at.%) as a base composition and other alloys with Mo up to 9 at. % and Mn up to 42 at.% by replacing some of the elements in the base alloy. These alloys were equilibrated at temperatures from 1173 K to 1473 K for up to two months. Microstructure analysis was done by FE-SEM, EPMA and EBSD. In case of the Fe-Cr-Ni ternary system, the σ phase in equilibrium with fcc-γ phase thermodynamically exists up to 1223 K, whereas it can exist up to 1473 K and 1373 K in the quaternary system with Mo and Mn, respectively. The increase in phase stability of the σ phase is interpreted in terms of the partition coefficients of M, *k*, among the three phases. In addition, the experimentally determined phase diagrams were reproduced by calculation using the modified thermodynamic database by assessing interaction parameters among the elements in each phase. Based on these results, microstructures with the s phase homogeneously precip-itated along the grain boundaries can be produced, indicating that the σ phase can be used as a strengthener of austenitic steels.

P–30

High pressure synthesis and thermoelectric properties of phases in the Eu-Al-Si system
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High-pressure, high-temperature synthesis can be used to access novel structural patterns, which, when quenched under pressure, remain thermodynamically metastable but indefinitely kinetically stable. For thermoelectric applications, such methods open the possibility to investigate the transport properties of new phases or polymorphs of known compounds. Here we report on the synthesis of compounds within the Eu-Al-Si system using pressures of up to 15 GPa and temperatures up to 1820 K. One such high pressure phase is the excess-electron clathrate, $EuSi_6$, which forms at pressures above 6 GPa, and remains metastable at ambient pressure up to 777 K. Motivated by a previous study showing that Ga is soluble on the Si site up to x=0.6 (in $EuGa_xSi_{6-x}$), here we investigate the solubility of Al on the Si site, with the goal of reducing the electron count to achieve semiconducting behavior and ultimately, improved thermoelectric performance. In addition, high pressure polymorphs of the Zintl phase $EuAl_2Si_2$ have been explored. Comparing the physical properties of such polymorphs can potentially provide insight regarding the influence of factors such as coordination number, bond length and polarity, and structural complexity on the electronic and thermal transport properties of intermetallic systems.

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Phase Equilibria among β/α_2/γPhases in γ-TiAl Alloys with Combined Addition of β-stabilizing Elements at 1073 K

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Phase equilibria among β-Ti (bcc), α_2-Ti_3Al ($D0_{19}$) and γ-TiAl (L_{10}) phases and the microstructure stability in Ti-Al-M_1-M_2 quaternary alloys (M: β-Tiphase stabilizing element) at 1073 K have been examined based on thermodynamic calculation and microstructure analyses, in order to evaluate the validity of our thermodynamic database accessed at 1373 K and 1473 K. The database used was first accessed to reproduce the experimentally determined phase diagramsat these two higher temperatures by calculation.Unlike the expectation from the two ternary systems of Ti-Al-$M_1$and Ti-Al-M_2, the combined addition of the M elements was found to stabilize the β phase, and this can be described by introducing negative interaction among the elements Al/M_1/M_2 in the β phase. By taking the composition and temperature dependence of the interaction parameters into account, the calculated phase diagrams aregood agreement withthe experimentally determined phase diagram. Then based on the calculated 1073 K phase diagram using the database, several quaternary alloys with various volume fractions of the β, α_2 and γ phases at 1073 K were selected.Note that these alloys have a unique transformation pathway of $\beta+\alpha \rightarrow \alpha \rightarrow \alpha(\alpha_2)+\gamma \rightarrow \beta+\alpha(\alpha_2)+\gamma$or β+γ during cooling, which makes it possible to hot-forge in processing and toughen in use. These alloys were hot forged and then employed to a specific two-step heat treatment to control the microstructure to nearly lamellar microstructure (NL). The specimen were then exposed at 1073 K for 2000 h. Some ofthe alloys exhibit a parlitic phase transformation ($\alpha_2+\gamma \rightarrow \beta+\gamma$) with a cellular morphology from the lamellar colony boundaries towar the lamellar grain interior during aging, indicating that the microstructure within the cell is clos to the equilibrium state. The quantitative analyses of the compositions and volume fractions of the β and γ phases within the cell are fairly in good agreement with those predicted from the calculated phase diagrams. This work was partially supported by the program of “Structural Materials for Innovation” in Cross-ministerial Strategic Innovation Program (SIP).

Notes

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