RUB

BOOK OF ABSTRACTS

MODELLING AND SIMULATION OF SUPERALLOYS

13+14 SEP. 2014: HANDS-ON TUTORIALS
15-17 SEP. 2014: INTERNATIONAL WORKSHOP
RUHR-UNIVERSITÄT BOCHUM, GERMANY

Organizers
Jutta Rogal, Thomas Hammerschmidt, Ralf Drautz

**Materials
Research
Department**

ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

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Modelling and Simulation of Superalloys

International workshop, 15-17 September 2014 and hands-on tutorials, 13-14 September 2014, Ruhr-Universität Bochum, Germany

Superalloys are multi-component materials with complex microstructures that offer unique properties for high-temperature applications. The complexity of the superalloy materials makes it particularly challenging to obtain fundamental insight into their behaviour from the atomic structure to turbine blades. Recent advances in modelling and simulation of superalloys contribute to a better understanding and prediction of materials properties and therefore offer guidance for the development of new alloys.

This workshop will give an overview of recent progress in modelling and simulation of materials for superalloys, with a focus on single crystal Ni-base and Co-base alloys. Topics will include electronic structure methods, atomistic simulations, microstructure modelling and modelling of microstructural evolution, solidification and process simulation as well as the modelling of phase stability and thermodynamics.

The workshop is organized by Jutta Rogal, Thomas Hammerschmidt and Ralf Drautz within the SFB/Transregio 103 Superalloy Single Crystals "From atoms to turbine-blades".

Workshop venue

The workshop will take place in the Conference Centre of the Ruhr-Universität Bochum (room 2a). It is located at the main campus below the mensa. It can be easily reached by public transport. A limited number of parking spaces are available in parking P9. You can reach the information desk of the Conference Centre at +49 234 32 25000.
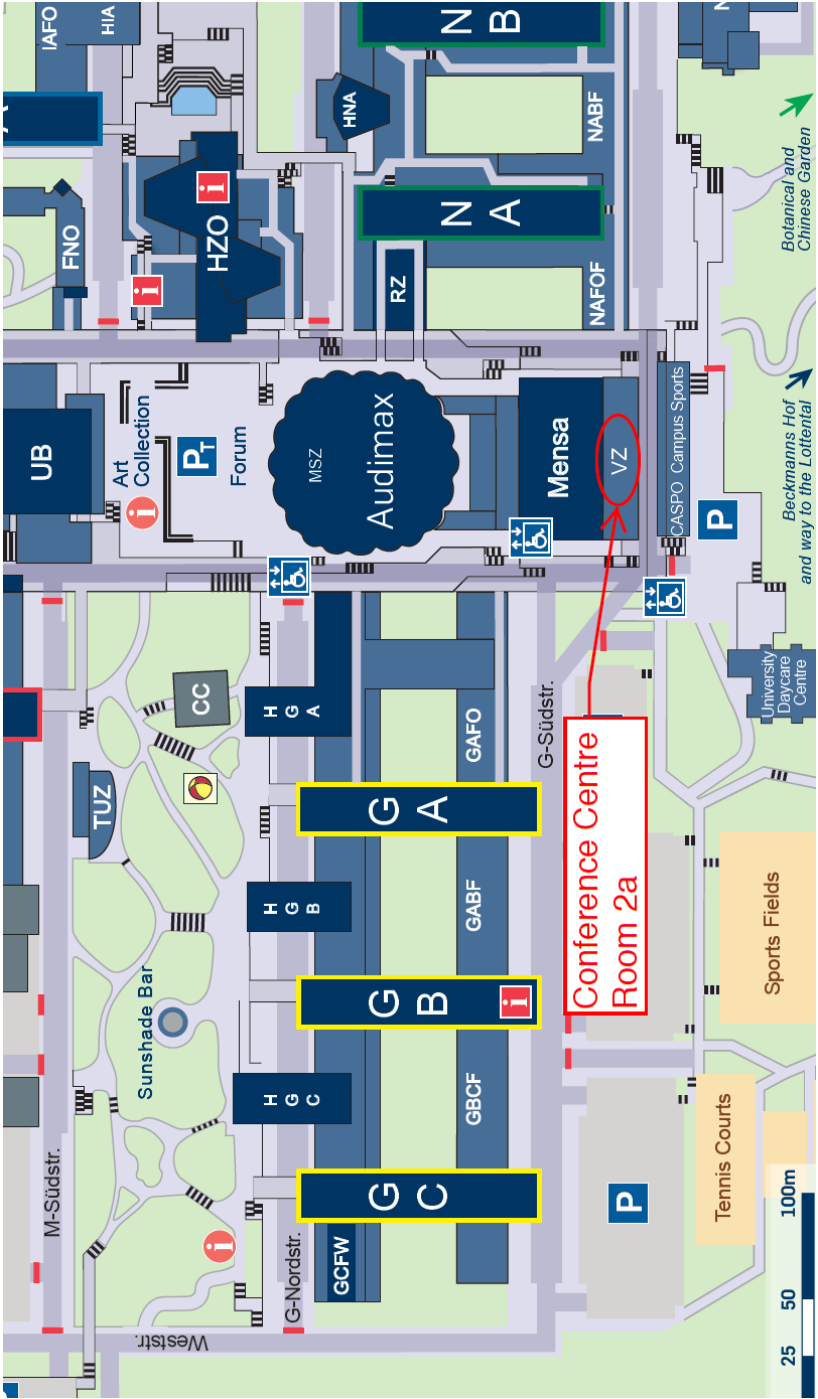
Travel Information

By public transport
Bochum Central Station is served by ICE, IC, EC, regional, and suburban trains at a high frequency. From there, you can reach us easily by taking the underground line U35 (CampusLinie) straight to the Ruhr-Universität Bochum (RUB). The U35 (direction Bochum Hustadt) runs at five-minute intervals on weekdays and takes just ten minutes to get to the university.

By car
Motorists can easily reach the RUB via the dense network of motorways in Germany and especially in North Rhine-Westphalia. The quickest route is via the motorway junction Bochum/Witten, where the A43 and A44 meet. Simply take the exit Bochum-Querenburg, follow the signs "Ruhr-Universität" and then the (electronic) information boards. A limited number of parking spaces are available in parking P9.

By plane
Four airports – Dortmund, Münster/Osnabrück, Cologne/Bonn, and Düsseldorf – are within a reasonable distance of the RUB. Düsseldorf Airport, however, is not only the largest, but also the most easily accessed: there are direct connections between the airport and Bochum's main train station up to eight times per hour, and the journey only takes around half an hour.

IAFO
HIA
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RZ
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Art Collection
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MSZ
Audimax
Mensa
VZ
CASPO Campus Sports
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Botanical and Chinese Garden
Beckmanns Hof and way to the Lottental
University Daycare Centre
CC
H G A
GAFO
G-Südstr.
TUZ
G A
H G B
GABF
Conference Centre Room 2a
Sunshade Bar
G B
GBCF
H G C
Sports Fields
M-Südstr.
G C
G-Nordstr.
GCFW
P
Tennis Courts
Weststr.

25   50   100m

Tutorials venue

The tutorials will take place at ICAMS in the building IC in room IC 02/718. Please make sure that you arrive in time for the tutorials, as the university is closed on the weekend and we have to let you in the building.

Travel information

From the Bochum Central Station you can reach ICAMS by taking the underground line U35 (CampusLinie, direction Bochum Hustadt) to the stop „Lennershof" (one stop after Ruhr-Universität Bochum). The U35 runs at ten-minute intervals on weekends and takes just eleven minutes to get to „Lennershof".

From Lennershof to IC, I-Nordstraße:

1. Head southeast on "Im Westenfeld" toward "Uhlenbrinkstraße" (130m) ,
2. Turn right onto "Zum Schebbruch" (180 m),
3. Turn left onto "Lennershofstraße" (96 m),
4. Turn right toward "I-Nordstraße" (18 m),
5. Turn right onto "I-Nordstraße" destination will be on the left (150 m).
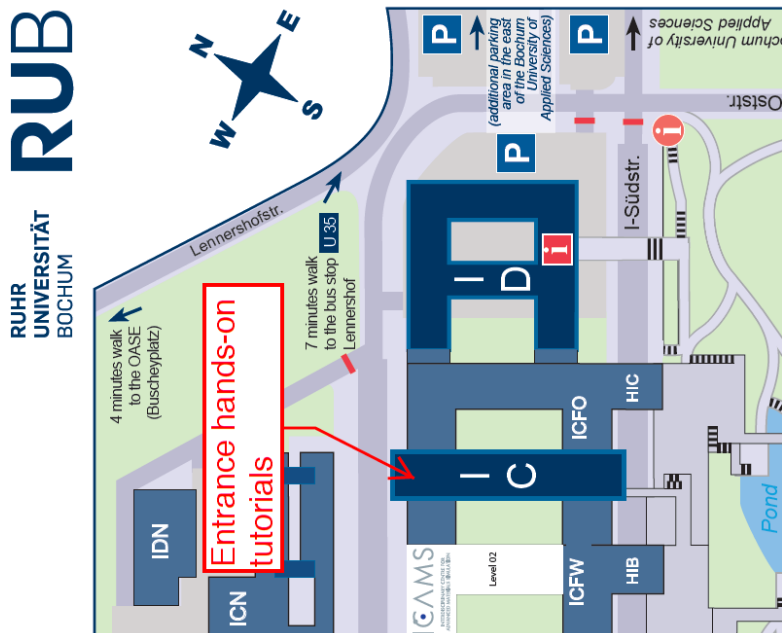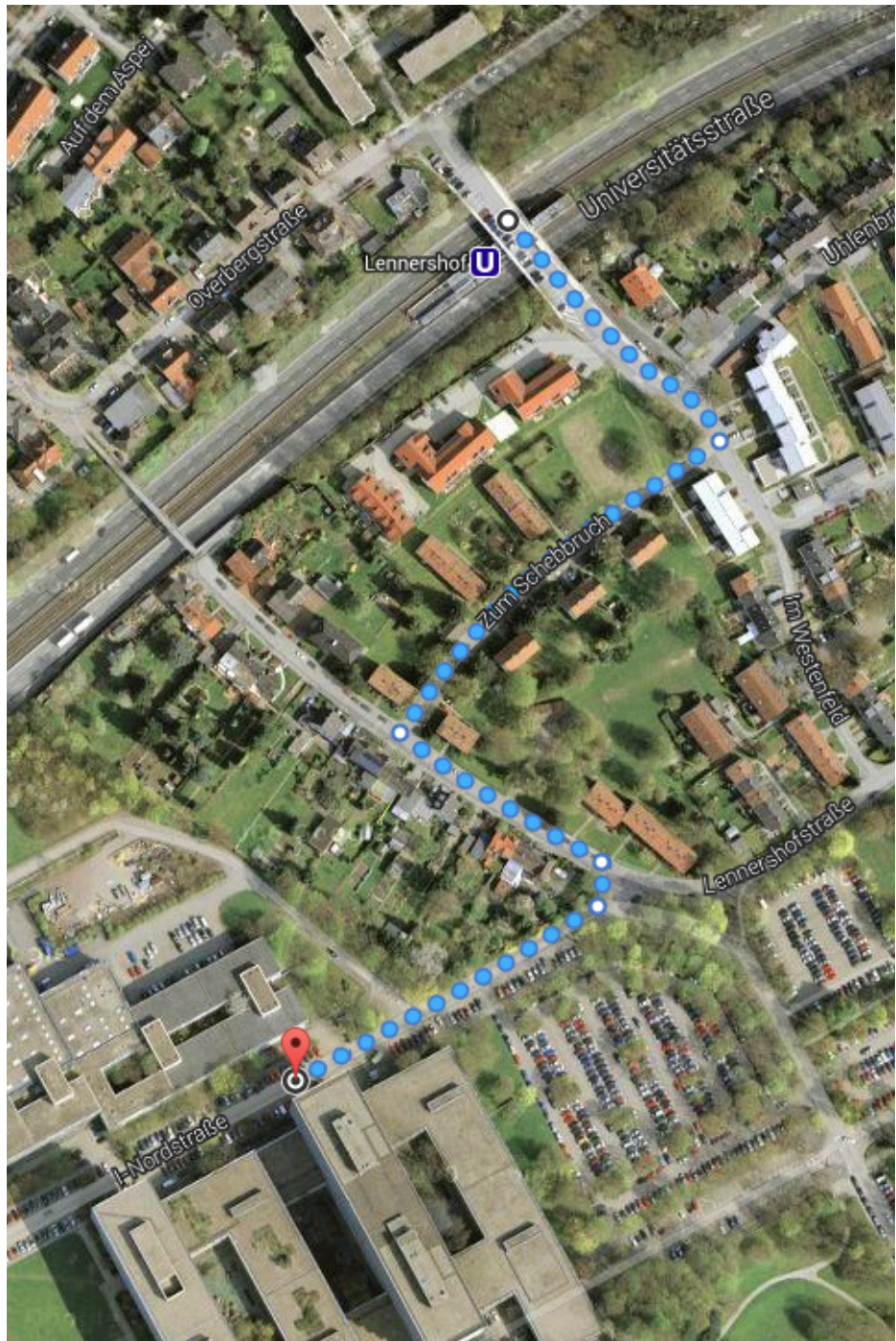
Conference Dinner

The conference dinner will take place at Restaurant Haus Herbede.

Von Elverfeldt-Allee 12, 58456 Witten,
Tel.: 02302/72258; Fax: 02302/79283,
http://www.restaurant-haus-herbede.de

Schedule Tutorials

In advance of the workshop we offer classes accompanied by hands-on tutorials on modelling and simulation of superalloys. The length scales relevant for superalloys from the electronic structure to continuum descriptions will be discussed and presented on a level accessible to interested graduate students and postdocs also with an experimental background. Participation in the tutorials will be limited to 50.

Tutorials and hands-on classes

*   Jörg Koßmann, Thomas Hammerschmidt - Modelling of phase stability with density functional theory

*   Sergej Schuwalow, Jutta Rogal - Diffusion properties from density functional theory

*   Juan Wang, Erik Bitzek - Atomistic simulation of dislocation properties

*   Siwen Gao, Anxin Ma - Discrete dislocation dynamics and crystal plasticity

*   Mohan Rajendran, Oleg Shchyglo - Phase field modelling of precipitation and ripening

*   Mauro Palumbo, Suzana Fries - Thermodynamic modelling using CALPHAD and density functional theory

Schedule

Saturday 13 September 2014

 8:30 - 9:15 registration

 9:15 - 10:00 lecture Koßmann
10:15 - 11:45 hands-on Koßmann, Hammerschmidt

11:45 - 13:00 lunch (will be provided)

13:00 - 13:45 lecture Rogal
14:00 - 15:30 hands-on Rogal, Schuwalow

15:30 - 16:00 coffee

16:00 - 16:45 lecture Bitzek
17:00 - 18:30 hands-on Bitzek, Wang

Sunday 14 September 2014

 9:15 - 10:00 lecture Ma
10:15 - 11:45 hands-on Ma, Gao

11:45 - 13:00 lunch (will be provided)

13:00 - 13:45 lecture Shchyglo
14:00 - 15:30 hands-on Shchyglo, Rajendran

15:30 - 16:00 coffee

16:00 - 16:45 lecture Palumbo
17:00 - 18:30 hands-on Palumbo, Fries

Schedule Workshop

Monday, September 15

9:30	MRD members assembly (for members of the Materials Research Department only)
12:00	Registration
13:30	Jutta Rogal, Thomas Hammerschmidt, Ralf Drautz, *Welcome*
13:45	Gunther Eggeler, *Recent progress in the microstructural understanding of high temperature and low stress creep of single crystal Ni-base superalloys* (invited)
14:30	Marc Fivel, *Initial stage of creep in Ni Superalloys: a 3D discrete dislocation dynamics investigation* (invited)
15:15	Coffee break
15:45	Yunzhi Wang, *Modeling Precipitate-Dislocation Interactions in Ni-Base Superalloys* (invited)
16:30	Masood Hafez Haghighat, *Characterization and modeling of the propagation of creep dislocations from the interdendritic boundaries in single crystal Ni base superalloys*
16:55	Mohan Kumar Rajendran, *A meso-scale approach to superalloys microstructure modeling*
17:20	Close
17:30 - 20:00	Poster session Discussion time with snacks and drinks

Tuesday, September 16

9:00	Erdmann Spiecker, *New approaches for quantitative analysis of single crystal superalloys based on advanced transmission electron microscopy* (invited)
9:45	James Kermode, *Multiscale modelling of materials chemomechanics: from brittle fracture in ceramics to dislocation motion in superalloys*
10:10	Juan Wang, *Atomistic Simulations of Dislocation-Interface Interactions in the γ/γ' Microstructure in Ni-based Superalloys*
10:35	Coffee break
11:05	Anton Van der Ven, *First-principles thermodynamics and kinetics of high temperature materials* (invited)
11:50	Kamal Nayan Goswami, *Can slow-diffusing solute atoms reduce vacancy diffusion in Ni-based superalloys?*
12:15	Sergej Schuwalow, *Vacancy mobility and interaction with transition metal solutes in Ni*
12:40	Lunch (on your own)
14:00	Pyuck-Pa Choi, *Characterization of Ni- and Co-based superalloys using Atom Probe Tomography* (invited)
14:45	Chris Wolverton, *Strength and Stability of $Co_3(Al,W)$ $L1_2$ γ'* (invited)
15:30	Coffee break
16:00	Alessandro Mottura, *Planar faults energies in multicomponent Co-base superalloys* (invited)
16:45	Sri Raghunath Joshi, *Partitioning and sublattice preference of alloying additions in $Co-Co_3W$ system*
17:10	Jörg Koßmann, *TCP precipitates in Co-based superalloys studied with atomistic calculations*
17:35	Close
18:30	Departure for dinner
22:30	Return from dinner

Wednesday, September 17

9:00	Alfred Ludwig, *Exploration of ternary subsystems of superalloys by high-throughput thin film experimentation* (invited)
9:45	Nathalie Dupin, *Thermodynamic modelling of the γ and γ' phases in the Calphad approach* (invited)
10:30	Jian Peng, *Experiment and Thermodynamic Assessment of the Al-Ni-Mo System*
10:55	Coffee break
11:25	Yuri Mishin, *Atomistic modeling of γ - γ' alloys* (invited)
12:10	Stefan Müller, *Structure and stability of Ni-rich alloys based on quantum mechanics* (invited)
12:55	Lunch (on your own)
14:30	Nicholas Hatcher, *Integrated Computational Materials Design (ICME) of Co- and Ni-based superalloys*
14:55	Ralf Rettig, *Single-crystal nickel-based superalloys developed by numerical multi-criterion optimization techniques based on thermodynamic calculations*
15:20	Jutta Rogal, Thomas Hammerschmidt, Ralf Drautz, *Concluding remarks*
15:30	Coffee break
16:00	Close of workshop

Abstracts talks

Recent progress in the microstructural understanding of high temperature and low stress creep of single crystal Ni-base superalloys

A. Basir Parsa, C. Somsen, A. Kostka, P. Wollgramm, H. Buck, K. Neuking, G. Eggeler

Institut für Werkstoffe, Ruhr-Universität Bochum

Single crystal Ni-base superalloys (SX) have a microstructure which consists of ordered cuboidal γ' particles (L1$_2$ phase, 70 vol.%, cube edge length: 0.5 micrometer) which are separated by thin γ channels (fcc, 30 vol. %, channel width: 0.1 micrometer). The response of SX to constant stress tensile loading is a creep rate, which strongly depends on microstructure. During creep the microstructure evolves. Particles coarsen and the subtle details of dislocation plasticity govern deformation behavior. A brief introduction into the elementary mechanisms of high temperature plasticity is given. Recent progress in the microstructural understanding is presented, addressing the high temperature and low stress creep anisotropy and the interaction between plasticity and rafting. Areas in need of further work are pointed out.

Monday, September 15

Initial stage of creep in Ni Superalloys: a 3D discrete dislocation dynamics investigation

Marc C. Fivel*, Jean-Loup Strudel, Hyung-Jun Chang

Univ. Grenoble Alpes / CNRS, SIMaP-GPM2

For low applied stresses, 2-phase γ-γ′ Ni superalloys display an abnormal behavior often referred to as negative creep. This surprising stage in the plasticity behavior corresponds to a contraction of the specimen length under tensile loading conditions. It results as the sum of two opposite contributions: the plastic creep strain associated with the area swept by dislocations within the narrow Ni matrix channels normal to the applied stress and the elastic relaxation they provide to the large internal stresses induced by the γ-γ′ lattice misfit in these channels. In this presentation, negative creep of Ni superalloys is investigated using 3D discrete dislocation dynamics (DDD) modeling. The simulated volume corresponds to a 3D periodic cell of an array of γ′-Ni_3Al cuboids ideally aligned in a γ matrix and loaded along the (001) direction. Misfit stresses induced by the γ-γ′ lattice mismatch ($d=-3.10^{-3}$) is taken into account through a coupling of the DDD code with finite elements.

Monday, September 15

Modeling Precipitate-Dislocation Interactions in Ni-Base Superalloys

Duchao Lv, Don McAllister, Michael Mills, Yunzhi Wang

The Ohio State University

Because of the multitude of deformation mechanisms operative at service temperatures and the strong influence of microstructure on the deformation modes in Ni-base superalloys, development of predictive property models requires incorporation of specific deformation mechanisms operating in specific alloy systems under a given set of microstructure states and service conditions. In this presentation, we show the use of phase field method in combination with experimental characterization and ab initio calculations in an attempt to identify deformation mechanisms and quantify activation pathways of precipitate shearing in Ni-base superalloys. In particular, deformation mechanism maps are established based on the simulation results, which could be incorporated in crystal plasticity models. Effects of microstructural features beyond average particle size and volume fraction of precipitates, such as precipitate shape and spatial distribution, on mechanical properties are also quantified.

Monday, September 15

Characterization and modeling of the propagation of creep dislocations from the interdendritic boundaries in single crystal Ni base superalloys

S.M. Hafez Haghighat, Z. Li, S. Zaefferer, R.C. Reed, D. Raabe

Max-Planck Institute for Iron Research, University of Oxford

In Ni base superalloys the initial dislocation density is always found to be very low, as observed for example using transmission electron microscopy. During the creep process the essentially dislocation-free regions are gradually percolated by multiplication of dislocations from sources, the origin of which have not been well understood. Interdendritic boundaries are known to exist in the as-cast structure of single crystal Ni base superalloys. In this study electron channeling contrast imaging (ECCI) is used to characterize the geometrically necessary dislocations (GND) at the interdendritic boundaries. Discrete dislocation dynamics (DDD) simulation is used to model the propagation of the dislocations from the interdendritic boundaries through the γ-γ' microstructure of Ni base superalloys. The modeling approach allows the necessary contributions of dislocation climb process to the dislocation flow. Insights into the role played by the interdendritic boundaries are provided.

Monday, September 15

A meso-scale aproach to superalloys microstructure modeling

M.K. Rajendran, J.V. Görler, O. Shchyglo, I. Steinbach.

Scale Bridging Thermodynamic and Kinetic Simulation, ICAMS, Ruhr-Universität Bochum

Ni-base superalloys show a superior strength at elevated temperatures because of their precipitation hardening by the γ' [Ni_3 (Al, Ti)] phase in γ-phase matrix. It is known that the mechanical properties strongly depend on the distribution and size of the precipitates. Knowledge of the precipitate growth kinetics and identifying the controlling parameters is an important aspect of the design and development of superalloys. The present research work is directed towards the study of superalloys microstructure evolution during heat treatment and high temperature applications withing the framework of the SFB/TR103 "Superalloy Single Crystals". We study γ-γ' microstructure under various conditions by a large scale three-dimensional phase field simulation. The microstructure evolution during different heat treatment cycles and under service conditions are numerically simulated using our in-house open-source library OpenPhase.

Monday, September 15

New approaches for quantitative analysis of single crystal superalloys based on advanced transmission electron microscopy

Erdmann Spiecker, Julian Müller, Yolita-Maria Eggeler

Center for Nanoanalysis and Electron Microscopy (CENEM), Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg

In this contribution we present new approaches based on advanced TEM techniques and FIB technology for investigating key aspects of the γ-γ' microstructure which govern the creep behavior of Ni- and Co-based superalloys. (i) A fully reliable technique for determining the complete Burgers vector of superdislocations by means large-angle convergent beam electron diffraction (LACBED) is demonstrated. (ii) A site-specific FIB preparation is devised which enables atomic resolution studies of the core structure of preselected superdislocations. (iii) An automized STEM-CBED-EDX technique for combined mapping of local strain fields and chemical composition in the γ-γ' microstructure is demonstrated. (iv) In situ TEM heating experiments are shown to be capable of addressing temperature dependent structural properties, like γ-γ' lattice misfit and phase stability. The different techniques are discussed with respect to their potential to contribute quantitative data for computational studies.

Tuesday, September 16

Multiscale modelling of materials chemomechanics: from brittle fracture in ceramics to dislocation motion in superalloys

James Kermode, Federico Bianchini, Giovanni Peralta, Zhenwei Li, Marco Caccin, Alessandro De Vita

King's College London

The underlying failure processes in many materials are surprisingly poorly understood, because of the complex chemistry invariably involved at the nanoscale. Jet engines are a prominent example, with their maximum operating temperature (and hence efficiency) limited by creep in their superalloy turbine blades. The 'Learn on the Fly' (LOTF) approach is a multiscale QM/MM coupling scheme that allows these kinds of "chemomechanical" processes - where long-range stress and local chemistry are tightly coupled - to be modelled with QM precision. The scheme has been applied to model a number of materials failure process in covalent materials and oxides, and has very recently been expanded to metals. I will give an overview of the approach and recent applications, with emphasis on a current project on the mechanical properties of Ni-based superalloys.

Tuesday, September 16

Atomistic Simulations of Dislocation-Interface Interactions in the γ/γ' Microstructure in Ni-based Superalloys

J. Wang, J. Guénolé, A. Prakash, E. Bitzek

Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Materials Science & Engineering, Institute I

The interaction of dislocations in the channels with the γ' precipitates is a main factor for the superior strength of Ni-based superalloys even at high temperatures. Here we report on a detailed study of screw and 60° dislocations interacting with a planar γ/γ'-interphase boundary in a quasi-two dimensional set-up. Static calculations as well as molecular dynamic calculations were performed to determine the critical penetration stress and to study the interaction of the channel dislocations with the misfit dislocation network. In addition, the interaction of dislocations with a curved interphase boundary was studied in a fully 3D set-up modeling an experimental microstructure obtained by 3D Atom Probe Tomography. The results of the simulations are discussed in the framework of a multiscale modeling approach to study the mechanical behavior and stability of Ni-based superalloys.

Tuesday, September 16

First-principles thermodynamics and kinetics of high temperature materials

Anton Van der Ven

University of California Santa Barbara

Predicting high temperature thermodynamic and kinetic properties of technologically important materials from first principles remains a major challenge. Most materials of practical interest are multi-component and exhibit varying degrees of long and short-range order. In addition to configurational disorder, anharmonic vibrational excitations can also be important in determining high temperature thermodynamic properties and must be accounted for in the description of a subset of structural phase transitions. The complexity of solid-state diffusion also increases with the number of components in the solid. Effective Hamiltonians parameterized from first principles allow for a systematic treatment of relevant excitations within statistical mechanical predictions of finite temperature thermodynamic, mechanical and kinetic properties of solids. In this talk I will illustrate this approach as applied to a variety of technologically important alloys.

Tuesday, September 16

Can slow-diffusing solute atoms reduce vacancy diffusion in Ni-based superalloys?

Kamal Nayan Goswami and Alessandro Mottura

University of Birmingham

The high-temperature mechanical properties of Ni-based superalloys can be heavily influenced by adjusting the chemical composition. The widely-accepted argument is that under certain temperature and loading conditions, plasticity occurs only in the γ matrix, and dislocations have to rely on thermally-activated climb mechanisms to overcome the barriers to glide posed by the γ' precipitates. The presence of dilute amounts of slow-diffusing solute atoms, such as Re, in the γ matrix is thought to reduce plasticity by retarding the climb of dislocations at the γ/γ' interface. One hypothesis is that the presence of these solutes must hinder the flow of vacancies, which are essential to the climb process. In this work, density functional theory calculations were used to inform an analytical model to describe the effect of solute atoms on the diffusion of vacancies. Results suggest that slow-diffusing solute atoms are not effective at reducing the diffusion of vacancies in these systems.

Tuesday, September 16

Vacancy mobility and interaction with transition metal solutes in Ni

Sergej Schuwalow, Jutta Rogal, Ralf Drautz

ICAMS, Ruhr-Universität Bochum

The dependence of high-temperature properties of Ni-based superalloys on the alloying additives is a subject of ongoing research. Current knowledge is mostly phenomenological in nature and the details of solute diffusion, interaction with defects, and the interplay between composition and microstructure are not well understood. Within this work interaction of Re, Ta, W and Mo solutes with vacancies and their diffusion in fcc Ni is investigated by density-functional theory (DFT) in combination with kinetic Monte Carlo (kMC) simulations. We calculate solute-vacancy interaction energies and macroscopic diffusion coefficients for the four elements in Ni as well as for vacancies themselves in the presence of these elements. The calculated solute diffusion coefficients are found to compare favorably to experimental values. The mobility of the vacancies as a key factor in dislocation climb is found to be only minimally influenced by the solute atoms within the dilute limit.

Tuesday, September 16

Characterization of Ni- and Co-based superalloys using Atom Probe Tomography

P. Choi[1], I. Povstugar[1], Z. Peng[2], K. Matuszewski[2], A. Rettig[2], R. Singer[2], S. Neumeier[2], C. Zenk[2], A. Bauer[2], M. Göken[2], D. Raabe[1]

[1] *Max-Planck-Institut für Eisenforschung,*
[2] *Friedrich-Alexander-Universität Erlangen*

We use Atom Probe Tomography (APT) for studying elemental distributions and partitioning in Ni- and Co-based superalloys and for addressing two topics. The first topic is on the characterization of Co-Al-W-Ti-Ta superalloys. We detect partitioning of all solute elements (Al, W, Ti, Ta) to the γ'-phase. Local nanoindentation testing on γ'-precipitates and γ-channels show that there is a hardness increase of γ' upon alloying with Ti and/or Ta and that it can be ascribed to the substitution of Al and W atoms by these elements. The second topic deals with the effect of Ru on suppressing the formation of deleterious TCP phases in Ni-based superalloys. We comparatively study two different alloys, Astra 1-20 (Ru-free) and Astra 1-21 (1% Ru) upong long-term aging. We show that Ru partitions to the TCP and γ phase, while it does not alter partitioning of other alloying elements. No interfacial segregation is observed. Possible mechanisms of the "Ru effect" are discussed based on the APT data.

Tuesday, September 16

Strength and Stability of $Co_3(Al,W)$ L1$_2$ γ'

James Saal, Chris Wolverton

Northwestern University

Although Co-based superalloys are considered as a promising next-generation turbine blade material, there are critical issues concerning poor high-temperature mechanical properties and phase stability that must be addressed before practical application is possible. We explore the fundamental properties for the base $Co_3(Al,W)$ L1$_2$ γ' using density functional theory. We have predicted the thermodynamic stability of $Co_3(Al,W)$ γ' and found that at low temperatures, γ' is a thermodynamically metastable phase. At higher temperatures, entropy-driven effects may potentially stabilize the structure. We have also predicted the antiphase boundary (APB) energies, a fundamental thermodynamic quantity that influences the high-temperature yield strength anomaly. The Al/W composition dependence of 100 and 111 APB energies are explored for $Co_3(Al,W)$ L1$_2$ γ'. From these results, we suggest possible methods for improving mechanical properties and phase stability in γ', particularly from alloying.

Tuesday, September 16

Planar faults energies in multicomponent Co-base superalloys

Alessandro Mottura

School of Metallurgy and Materials, University of Birmingham

Creep deformation mechanisms markedly change with chemistry in the superalloys. The planar faults observed after creep in Co-based superalloys are dramatically different to the planar faults observed after creep in Ni-based superalloys. This happens, in part, due to the effect of chemistry on planar fault energies. In this work, using a variety of modeling methods, the variation of planar fault energies across wide compositional ranges in multi-component Co-based alloys is investigated. Results are discussed in light of high-resolution energy dispersive spectroscopy and high-resolution scanning transmission electron microscopy results showing segregation of elements such as Ta and W to the superlattice intrinsic stacking faults. Although Ta additions may produce an increase in stacking fault energies, the presence of other solute elements can lead to synergetic effects, which instead minimize the value of stacking fault energies.

Tuesday, September 16

Partitioning and sublattice preference of alloying additions in Co-Co$_3$W system

Sri Raghunath Joshi, K. V. Vamsi and S. Karthikeyan

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

Recent interest in Co-base superalloys has been due to the discovery of cubic L1$_2$ precipitates in the Co-Al-W system. However, the γ+γ′ phase field is stable only over a narrow range of compositions and thus there is a need for exploring alternative alloy systems. This study was aimed at probing the role of alloying on stability of Co$_3$W precipitates via electronic structure calculations based on density functional theory. Ground-state energies and lattice parameters were computed for fcc Co and Co$_3$W (in L1$_2$ and D0$_{19}$ structures) alloyed with X = Mn, Fe, Ni, Pt, Cr, Al, Si, V, W, Ta, Ti, Nb, Hf, Zr and Mo. In the ordered structures, these alloying elements were substituted into both sublattices. The aim was to evaluate the preference of X for the Co sublattice in L1$_2$ and D0$_{19}$, W sublattice in L1$_2$ and D0$_{19}$ and fcc Co solid solution. Results suggest that alloy partitioning derived from sublattice preference can be used for designing novel alloy compositions with dual phase microstructure.

Tuesday, September 16

TCP precipitates in Co-based superalloys studied with atomistic calculations

Jörg Koßmann, Thomas Hammerschmidt, Ralf Drautz

ICAMS, Ruhr-Universität Bochum

Since Sato et al. first observed a $L1_2$ phase in the ternary Co-Al-W system, Co-based materials have been shown to be promising candidates for the next generation of superalloys. The precipitation of topologically close-packed (TCP) phases deteriorates the mechanical properties of superalloys. In order to study the stability of such precipitates in Co-base superalloys, we compute the formation energy of typical TCP phases in binary and ternary systems. Furthermore, we apply an empirical structure map to interpret experimental experimental results. Our work is part of the collaborative research center SFB/TR 103.

Tuesday, September 16

Exploration of ternary subsystems of superalloys by high-throughput thin film experimentation

Alfred Ludwig, D. König, D. Naujoks, C. Eberling,
S. Thienhaus, A. Savan, J. Frenzel

Institute for Materials, Ruhr-University Bochum

Ternary subsystems of Ni- and Co-based superalloys are explored by combinatorial and high-throughput methods. The materials systems to be investigated (Ni-Al-Cr, Cr-Ni-Re, Co-Ti-W, Co-Al-W) are deposited in the form of materials libraries by special magnetron sputter deposition methods. These materials libraries are subsequently processed at high temperatures (< 1100°C) and characterized by high-throughput experimentation methods (automated EDX, XRD, temperature-dependent resistance screening) in order to relate compositional information with structural properties. The talk will cover examples of the combinatorial exploration of ternary sub-systems of superalloys with regard to identifying unknown phases as well as to explore the compositional ranges of the different phases. Examples of up-scaling from thin film findings to the bulk are discussed. Furthermore, the oxidation behavior of superalloy subsystems, e.g. Ni-Al-Cr was studied by high-throughput methods.

Wednesday, September 17

Thermodynamic modelling of the γ/γ' phases in the Calphad approach

N. Dupin

Calcul Thermodynamique

Superalloys are multicomponent alloys getting most of their mechanical properties from the γ/γ' relationship. Calphad thermodynamic modelling has shown its ability to describe the complexity of phase equilibria in many different multicomponent alloys. In order to describe properly the superalloys, the crystallographic ordering between the γ and γ' phases needs to be taken into account. Different assumptions commonly used in order to perform such thermodynamic descriptions will be discussed, and in particular the input of FP results.

Wednesday, September 17

Experiment and Thermodynamic Assessment of the Al-Ni-Mo System

Jian Peng, Peter Franke, Hans J. Seifert

Institute for Applied Materials - Applied Materials Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

The intermetallic compound NiAl possesses attractive properties for high temperature structural applications, e.g. high melting point (1638°C), substantially lower density (5.7 g/cm^3) than that of Ni-based superalloys, high oxidation resistance, and good thermal and electrical conductivity. However, besides its poor ductility and fracture toughness at room temperature, the use of NiAl as a structural material suffers mainly from low strength and creep resistance at temperatures above 600°C. Fortunately, recent advancements in directional solidification of NiAl-Mo eutectics enable to produce in-situ fiber reinforced composite (NiAl matrix and Mo fiber) with an unprecedented level of fiber alignment and regularity, and the mechanical properties are greatly improved compared to intermetallic compound NiAl. This composite has been demonstrated as a potential candidate used for as specific hot section components of turbine engines, blades or buckets and vanes as well as nozzles.

Although three versions of thermodynamic assessment for the Al-Ni-Mo system have been reported, it is still necessary to re-assess it due to several limitations of previous ones: a) In the earliest assessment, all compounds were described as stoichiometric compounds. b) The second assessment was found to be inconsistent with experimental phase equilibrium data at 800°C, limiting its utility in phase-field modeling. c) Despite of the more complete descriptions of Al-Ni-Mo system, most of the invariant reaction temperatures are inconsistent with the experimental data in the latest assessment. d) None of them can reproduce a

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reliable description for NiAl-Mo quasi-binary system. Moreover, important improvements, such as the modeling of the order-disorder transition of bcc A2 and bcc B2 phases, are published, but absent in Al-Ni-Mo system. Therefore, a more accurate thermodynamic descriptions for Al-Ni-Mo system, particularly for the NiAl-Mo quasi-binary system is needed, which can support the design of alloy microstructures, microstructure modeling and thermodynamic modelling of higher order systems.

In the present work, key experiments are carried out to describe the Ni-Al-Mo section more accurately and the experimental results are taken into account in the present assessment. A substitutional-solution model is used to describe liquid, fcc, and bcc phases, while sublattice models are used to describe intermetallic phases. More importantly, the disordered bcc A2 and ordered bcc B2 phases are also modelled with single Gibbs free energy function, as well as the disordered fcc and ordered $L1_2$ phases. Calculated phase diagrams are compared with the experimental data.

Wednesday, September 17

Atomistic modeling of γ-γ' alloys

Y. Mishin

George Mason University, Fairfax, Virginia

This talk will present an overview of recent atomistic computer simulations of γ-γ' structures in the Ni-Al system as well as ternary systems such as Ni-Al-Co and Ni-Al-Cr. The topics to discuss will include: (1) challenges in the development of interatomic potentials for the Ni-Al and Ni-Al-X systems; (2) thermodynamics of phases and calculation of phase diagrams for γ-γ' systems; (3) point defects in the γ' phase; (4) modeling of the atomic structure of coherent and incoherent γ-γ' phase boundaries; (5) calculation of the γ-γ' interface thickness and interface free energy: the capillary fluctuation method, effect of alloying, temperature and applied mechanical stresses; (6) local disordering (wetting transitions) at anti-phase boundaries in the γ' phase. Recent achievements, limitations and future directions in atomistic modeling of superalloys will be discussed.

Wednesday, September 17

Structure and stability of Ni-rich alloys based on quantum mechanics

S. Maisel, N. Schindzielorz, M. Höfler, S. Müller

Hamburg University of Technology, Institue of Advanced Ceramics

The characterization of Ni-rich alloys as function of the local environment (e.g. bulk concentration, temperature) is an important prerequisite for our understanding of Ni-based superalloys. We investigated different binary Ni-based alloys by means of density functional calculations combined with the cluster expansion method and Monte-Carlo simulations. Here, Ni-W and Ni-Re play an important role: While not as potent in its toughening as Re, W still is a prototypical superalloy strengther. It will be demonstrated that both alloy systems possess completely different ordering phenomena which makes the difference in their mechanical properties understandable. Interestingly, for higher temperatures even hcp-based structures can be stabilized in Ni-Re alloys, in agreement with recent experimenal data. It also will be shown, how the cluster expansion as realized by our computer code UNCLE can be applied for ternary and even quaternary alloy systems.

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Integrated Computational Materials Design (ICME) of Co- and Ni-based superalloys

Nicholas Hatcher, Jiadong Gong, David Snyder, Jason Sebastian, Greg Olson

QuesTek Innovations LLC

ICME within the US-MGI program has been applied to two superalloy systems: a high-strength, wear-resistant material alternative to Cu-Be for highly loaded, unlubricated aerospace bushing applications and a Ni-based single crystal (SX) superalloy for use in industrial gas turbine (IGT) blades. To avoid health-hazards associated with Be in Cu-Be, Co-based designs were developed to encourage $FCC/L1_2$ lattice parameter matching, and a final alloy design achieved desired properties with initial full scale prototypes produced. For advanced power plant technologies novel turbine blade materials were developed to exhibit the requisite creep rupture resistance. Designs address solutions to casting defects such as freckling, high/low angle boundary (HAB/LAB) formation, grain nucleation, and shrinkage/porosity. The design process included a systems approach with modelling, targeted experimental validation and characterization, and accelerated scale-up and manufacturing.

Wednesday, September 17

Single-crystal nickel-based superalloys developed by numerical multi-criterion optimization techniques based on thermodynamic calculations

Ralf Rettig, Nils Ritter, Alexander Müller, Harald Helmer,
Robert F. Singer

*Friedrich-Alexander-University Erlangen-Nürnberg,
Institute for Science and Technology of Metals*

A method for finding the optimum alloy compositions considering a large number of property requirements and constraints by systematic exploration of large composition spaces is proposed. This Computational Alloy Development can greatly enhance traditional trial-and-error testing. It is based on a numerical multi-criterion global optimization algorithm (Sequential Quadratic Programming), which delivers the exact optimum considering all constraints. The CALPHAD-method is used to provide the thermodynamic equilibrium properties of the alloys and the creep strength of the alloys is predicted based on a qualitative numerical model considering the solid solution strengthening of the matrix by the elements Re, Mo and W and the optimum morphology and fraction of the γ′ phase. The calculated alloy properties are provided via very fast Kriging surrogate models. The capability of the optimization is experimentally verified with two new single crystal compositions.

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Abstracts posters

Structural, electronic, magnetic and thermodynamic properties of full-Heusler compound Co$_2$VSi: Ab initio study

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Density functional theory based on full-potential linearized augmented plane wave (FP LAPW) method is used to investigate the structural, electronic and magnetic properties of Co$_2$VSi Heusler alloys, with L2$_1$ structure. It is shown that calculated lattice constants and spin magnetic moments are in good agreement with experimental values using the general gradient approximation method. We also presented the thermal effects using the quasi-harmonic Debye model, in which the lattice vibrations are taken into account. Temperature and pressure effects on the structural parameters, heat capacities, thermal expansion coefficient, and Debye temperatures are determined from the non-equilibrium Gibbs functions.

Poster session

Multiscale Atomistic Simulations of Ni-base Superalloys

F. Bianchini, J. R. Kermode and A. De Vita

King's College London, Physics Department

We are studying the mechanical properties of Ni-base superalloys using a multiscale quantum mechanical / molecular mechanical (QM/MM) approach. The main goal is understanding dislocation motion at the atomic-scale, especially near γ-γ' interfaces. We are using the `Learn on the Fly' (LOTF) technique [1], a multiscale method augmented by learning algorithms. Detailed convergence tests reveal that accurate forces can be achieved using only modest-sized clusters for the embedded QM calculations. The project was recently awarded a substantial PRACE award, enabling large-scale QM-accurate simulations of dislocation motion to be carried out for the first time [2].

[1] G. Csanyi, T. Albaret, M. Payne, and A. De Vita. Phys. Rev. Lett., 93:175503, 2004.
[2] J. R. Kermode, F. Bianchini, A. Comisso and A. De Vita, Multiscale Atomistic Simulation of the Mechanical Behaviour of Nickel-based Superalloys, 8th PRACE Project Access Call (awarded Feb 2014).

Poster session

First-principles study of the mechanical behaviour of Nickel and Nickel-rich alloys subject to [001] loading

A. Breidi[1], M. Palumbo[1], S. G. Fries[1], A. Ruban[2]

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Recent developments in materials engineering, such as the production of new generation Ni base superalloys that exhibit excellent mechanical strength, have stimulated interest in studies of the theoretical strength which in these materials may control both the onset of fracture and the dislocation nucleation. Inspired by that we apply quantum-mechanical calculations, namely coherent potential approximation and VASP methods, to the elemental fcc Ni and Ni-rich alloys, to examine their response to extreme loading conditions such as uniaxial compressive and tensile tests, aiming to identify their theoretical strength. We examine the elasticity at every applied strain, in order to explore a possible mechanical instability that may occur prior to reaching the material's ideal strength. The results can help in understanding the role of various transition metal elements, with particular emphasis on Re, on enhancing the solid solution strengthening mechanism.

Poster session

High temperature elastic properties and lattice misfit investigations of nickel-base superalloys ERBO1 and LEK94

Kathrin Demtröder[1], Hinrich Buck[2], Philip Wollgramm[2] and Jürgen Schreuer[1]

[1]*Institute for Geology, Mineralogy and Geophysics,*
[2]*Institute for Materials, Chair for Materials Science and Engineer*

The mechanical behavior of single crystal nickel-base superalloys depend on the one site on the chemical composition and on the other side on the microstructural change during their special operation conditions in gas turbines and turbine blades at high temperature. For this reason we employed resonant ultrasound spectroscopy (RUS) to study the elastic and anelastic behavior of ERBO1 and LEK94 between room-temperature and 1250°C. ERBO1 is a special superalloy, which is based on a CMSX-4 master melt and in the following a specific cast and heat treatment process were performed. Additionally, macroscopic creep experiments at 850°C with 620 MPa and at 1050°C with 160 MPa in the <001> loading direction were performed. The microstructural characterization of the samples was achieved by a combination of reciprocal space mapping, electron diffraction techniques (SEM, TEM), electron microprobe analysis, atomic force microscopy (AFM) and optical microscopy.

All samples show a pronounced sound attenuation above about 800°C, which is probably related to the gradual dissolution of the γ'-precipitates and could be a hint for an increasing number of point defects. Furthermore, the thermal treatment leads to significant changes of the microstructure, which in turn affects the elastic properties. Also the lattice misfit changed significantly after the creep experiments.

Poster session

Ab-Initio Study of Impurities Segregation Effects in Nickel Σ5 Grain Boundary

Bentria El Tayeb and Lefkaier Ibn Khaldoun

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We present in this work Ab initio calculation based on density functional theory of the effect of impurity on Nickel Σ5(012) symmetrical tilt grain boundary using Norm-conserving pseudopotentials (by setting niobium as an example). We first calculate segregation energies for interstitial and different substitutional sites, in order to determine site preferences and the segregation properties of Nb in Nickel GB. It is found that Niobium atoms prefer to segregate in substantial sites of the GB. Furthermore, calculations of tensile strength in Ni GB which have been preformed for the first time show an enhancement of the maximum tensile strength σMax mean that niobium acts as a strengthening element in Ni GB, which is in agreement with experimental observations.

Poster session

Extreme loading conditions in transition-metal disilicides: an ab initio study

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Transition-metal disilicides constitute a promising basis for a new generation of high-temperature structural materials that can significantly improve the thermal efficiency of energy conversion systems and advanced engines. Although they have been studied quite intensively, the complexity of their mechanical behavior is still not completely understood. Employing quantum-mechanical (ab initio) calculations of electronic structure, we investigate the effect of uniaxial loading for disilicides with hexagonal C40 structure, namely for $NbSi_2$, $CrSi_2$, VSi_2 and $TaSi_2$, and compare their behavior with previously studied $C11_b$ structure disilicides [1,2]. Further, the C40 structure disilicides are subjected to biaxial loading and the values of strains are extended up to their extreme levels, beyond materials stability limits represented here by the values of theoretical tensile strength. We find a direct correspondence between the electronic structure characteristics and the onset of strength instability.

[1] M. Friák, M. Šob, and V. Vitek: Ab initio study of ideal tensile strength and mechanical stability of transition-metal disilicides, Phys. Rev. B 68 (2003) 184101.
[2] M. Šob and M. Friák: The effect of structural degrees of freedom on bonding and strength characteristics of molybdenum disilicide, Intermetallics 17 (2009) 523.

Poster session

Going to finite temperature binary phase diagrams by exploring DFT and Bragg-Williams-Gorksy configuration entropy

M. Palumbo, J. Koßmann, T. Hammerschmidt,
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ICAMS, Ruhr-Universität Bochum

Poster session

Carbon Inclusions In Nickel-Titanium Alloys

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SAES Getters S.p.A, Italy

NiTi alloys are one of the most successful shape memory materials today used in fatigue rated devices. Inclusions content represents a serious concern for fatigue life. Typically, in NiTi alloys the inclusions are titanium carbides and intermetallic oxides.

In SAES Group we have developed a reliable procedure, combining SEM-EDS technique with optical metallography, for inclusion quantitative analysis in VIM/VAR NiTi alloys [1,2]. The inclusion type, size and amount have been observed to strongly depend on Ni/Ti ratio, melting and thermo-mechanical processes [3].

In this work, we provide an interpretation and a theoretical model for carbon inclusions formation in NiTi alloys by means of computational thermodynamics.

A strong chemical reactivity of graphite crucible with NiTi melt is demonstrated to be responsible of carbon diffusion and contamination during vacuum induction melting process. In Ni-rich formulations, titanium carbides represent the main precipitates. In Ti-rich formulations, carbides become nucleation centers of a $Ti_4Ni_2(C,O)$ phase, resulting in core-shell primary interdendrites.

[1] F. Sczerzenie et al., J. Mater. Eng. Perform., 2011, 20, 830
[2] A. Coda et al., J. Mater. Eng. Perform., 2012, 21, 2572
[3] F. Sczerzenie et al., J. Mater. Eng. Perform., 2012, 21, 2578

Poster session

Phase-field simulation of long term aging in Ni-base superalloys

Johannes V. Görler, Steffen Brinckmann,
Oleg Shchyglo, Ingo Steinbach

ICAMS, MPIE

Superalloys are of economic importance since they exhibit superior properties at elevated temperatures. However, Ni-Al alloys possess the unusual feature of having thin matrix-channels combined with a dominant precipitate phase. In this study, dislocation induced strains at the interface are used to describe coherent and semi-coherent interfaces. We find, that there is a driving force which prevents channel annihilation. Moreover, the presented study shows that in contrast to coherent interfaces, semi-coherent interfaces significantly reduce repulsive stresses in the γ-channels and promote channel annihilation and precipitate coalescence. This knowledge is then used in a phase field simulation to investigate the microstructure evolution during long term aging of Ni-base superalloys.

Poster session

Dislocation dynamics simulation of Ni base superalloy creep under different loading conditions

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Single crystal superalloys are used in the blades of advanced gas turbines, which operate in the creep range where they have to withstand mechanical loading at elevated temperatures. Creep is characterized by the evolution of strain with time, which limits service life of high temperature components. Most importantly, creep rates strongly depend on stress and temperature. It is well known that creep is governed by dislocation glide and climb processes which have been observed in the TEM and which are incorporated in micromechanical models. In the present study we use discrete dislocation dynamics (DDD) simulation to study the evolution of dislocations in a typical γ-γ' microstructure of a single crystal superalloy under different loading conditions. A hybrid glide-climb mobility model is used to conduct the interaction of dislocations with γ' particles. We focus on the early stages of creep, where dislocation plasticity is confined to narrow γ channels. In a first order approximation we assume that our system has no misfit and that the γ-γ' microstructure is stable. Using the implemented dislocation glide-climb mobility it appears that at elevated temperatures, i.e. when climb rates are high, the creep strains accumulated even for resolved shear stress which are smaller than the critical stresses required for dislocations to enter into the γ-channels. Simulated creep microstructure consists of long bent dislocations which form complex networks. At higher stresses, however, dislocations can penetrate the γ channels and deposit 60° mixed or screw dislocations at the γ-γ' interfaces. These observations are in a good agreement with previous experimental findings. In the present study an effort is also made to study the influence of crystallographic loading direction on creep.

<div align="center" style="color:red">Poster session</div>

Single-Crystal Solidification for Enhanced Microstructure:
Development of the FCBC Casting Process

Matthias Hofmeister, Ralf Rettig, Robert F. Singer

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Liquid Metal Cooling (LMC) struggles from the pollution of the ingot superalloy by the cooling agent in the case of mould crack during solidification. To overcome the drawback but still take advantage of the benefits in high gradient solidification like smaller dendrite arm spacing and reduced poresizes an advanced technique in investment casting is under development. The heat sink in the Fluidized Carbon Bed Cooling (FCBC) is provided by a fluidized bed applying carbon bed material agitated by inert gas. The fluidized bed allows the application of a free floating Dynamic Baffle. The layer of insulating particles assures an enhanced axial temperature gradient during solidification. High yield and improved mechanical properties are expected. Both, bed material and Dynamic Baffle, may be made from carbon material with is, when kept within limits, not a pollutant but an alloying element to the superalloy. Currently the attempt of FCBC is brought to prototype state.

Poster session

Topologically close-packed phases in Co- and Ni-base superalloys - Phase stability investigated with density functional theory and structure maps

J. Koßmann, T. Hammerschmidt, R. Drautz

ICAMS, Ruhr-Universität Bochum

Poster session

Theoretical Investigation of Superconductivity in Sr and Na Doped Graphene sheet

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Addis Ababa University, Materials Science Program

Graphene has many remarkable properties, but superconductivity is notably absent. Recent observation of proximity effect has ignited in superconductivity of graphene sheet. In this work we explore, using density functional theory (DFT) and density functional perturbation theory (DFPT) calculation the possibility of inducing superconductivity in strontium and sodium doped graphene. We have given a clear evidence that superconductivity critical temperature Tc is easily affected by the contribution of inplane phonon vibration of intercalate and outof- plane phonon (ZO) of the graphene sheet. Particularly Sr and Na intercalated graphene sheet leads to superconductivity, with $\lambda = 0.667$ with Tc of 7.5 K and 0.41 with Tc of 2 K for sodium and strontium intercalated graphene respectively.

Poster session

Modeling and Simulation of Heat Transfer phenomena during Investment casting

Muhammad Musaddique Ali Rafique, Javed Iqbal

Technische Universität Hamburg-Harburg, Germany

Determining the heat transfer phenomena during casting processes is an important parameter for measuring the overall performance of process. It gives information about the properties of the metal being casted and its possible behavior in the mold during casting process. Improper determination of heat transfer phenomena and use of improper molding materials and casting conditions leads to defects such as misruns, cold shuts, shrinkage, pin holes, air holes and porosity in final product. A mathematical model was developed using standard transport equations incorporating all heat transfer coefficients to calculate the time for solidification of metal in casting and computer simulation of the model was carried out in C++ to validate the model. The metal used was pure iron casted in investment molds of silica sand with zircon coating. It was shown that airflow near the mold surfaces was partially restricted due to geometry of the molds and arrangement of the pieces around a tree. So, the changes in heat transfer coefficient also contribute towards time of solidification. The time calculated was found to be in good agreement with experimental values.

Poster session

Electronic properties and diffusion behavior of refractory elements in Ni-base superalloys: a combined DFT+kMC approach

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Poster session