Scientific Report 2015 and 2016

ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS

Scientific Report

2015 and 2016

ICAMS
Ruhr-Universität Bochum
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44801 Bochum
Germany

Preface

Materials form the foundation on which technological progress is built. The availability of materials with improved properties and functionalities is critical for innovations in many sectors such as energy, environment, transport and health. The design of materials, compositions and microstructures to achieve specific characteristics requires a comprehensive description of materials from the fundamental laws of nature to engineering applications. This defines the mission of the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) at the Ruhr-Universität Bochum.

ICAMS is a leading centre of competence for scale-bridging modelling and simulation of materials. We provide materials-specific and problem-driven simulations to support a knowledge-based materials development.

This report gives a brief summary of the activities and achievements of ICAMS in 2015 and 2016. It summarizes the scientific interactions as documented by peer-reviewed publications and highlights other developments of relevance for ICAMS.

Ralf Drautz
Managing Director

Alexander Hartmaier
Director

Ingo Steinbach
Director

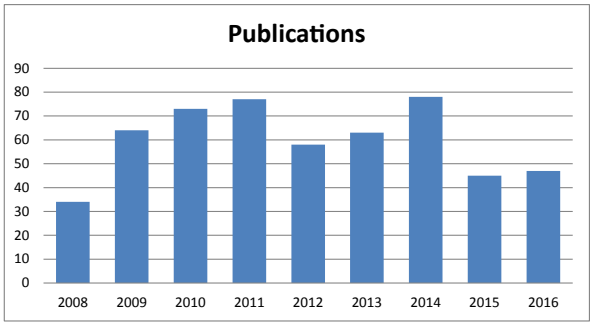
Contents

ICAMS in 2015 and 2016

2. ICAMS in 2015 and 2016

Publications

In 2015 and 2016 ICAMS researchers published 45 and 47 articles in peer-reviewed journals. In addition, the Advanced Study Groups listed 51 papers related to ICAMS in these two years. *Fig. 2.1* shows the number of publications and citations with ICAMS members as authors since 2008, according to Thomson Reuters' *Web of Science*. The number of publications shows a characteristic oscillation according to the typical three-year-duration of the PhD projects. In 2015 and 2016 24 PhD theses and 33 master theses have been completed at ICAMS.



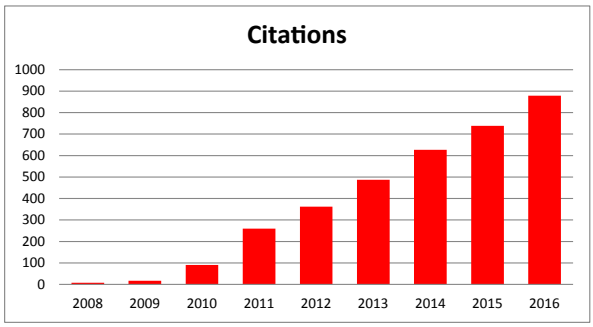


Fig. 2.1: ICAMS' publications, and citations since 2008. Citations are according to Thomson Reuters' Web of Science *in February 2017.*

Two large research projects characterized the work at ICAMS during the last two years. The ICAMS Demonstrator Project *Damage Tolerant Microstructures in Steel* was concluded in 2016. The second large project is the Collaborative Research Centre SFB/TR 103 *Superalloy Single Crystals*, with ICAMS leading the modelling activities.

Teaching

570 applications for the ICAMS Masters Course *Materials Science and Simulation* were received in 2015 and 2016. About 107 students were admitted, and 46 of them eventually took up their studies in the last two years. In total, 25 students completed their Master's degree. Most of them moved on to a PhD project or industry position in Germany. Other destinations of preference were the USA and several EU-countries. In addition, 8 theses from other master programmes have been supervised at ICAMS. The re-accreditation of the ICAMS Masters Course will take place in 2017.

Staff numbers and finances

In 2015 and 2016 about three quarters of the ICAMS staff were financed by third-party funding and approximately

one quarter by central funds of the Ruhr-Universität Bochum. Chapter 13 provides a detailed summary of the development of staff numbers in the past years. In the last two years more than 90% of the acquired third-party funds came from public funding agencies like the DFG and the EU and the rest from industry. As salaries and costs associated directly to staff (such as travel expenses etc.) constitute by far the largest expenditure of ICAMS, the staff numbers are approximately proportional to the average third-party income.

Workshops and conferences, outreach

ICAMS organised and contributed to the organisation of several workshops and conferences in the past two years. The *ICAMS Advanced Discussions* in June 2015 hosted international speakers, presentations from ICAMS members and the panel discussion 'From Atoms to Continuum'. The *Advanced Discussions* in May 2016 were dedicated to materials design from an experimental and theoretical point of view. The *25th International Workshop on Computational Mechanics of Materials* was organized by the Department of Micromechanical and Macroscopic Modelling in October 2015. The 2016 *Materials Day* in October was a joint workshop of the RUB Materials Research Department and the Max-Planck graduate school *SurMat*. In November 2016 the ICAMS department Micromechanical and Macroscopic Modelling took responsibility for the Trend-Workshop *Scalebridging Simulation: Material, Process, Component*.

Furthermore, ICAMS scientists were members of the scientific panels or contributed to the organization of the following conferences and workshops:

- SiMiDe Spring School, March 2015, Hamminkeln, Germany
- CALPHAD XLIV, May 2015, Loano, Italy
- International Workshop on Advanced Co-based Superalloys, June 2015, Gaithersburg, USA
- MCWASP XIV 2015, June 2015, Awaji Island, Japan
- PTM 2015, June 2015, Whistler, Canada
- ESMC 2015, July 2015, Madrid, Spain
- EUROMAT 2015 Symposium D3.2, September 2015, Warsaw, Poland
- Materials Chain International Conference - May/June 2016, Bochum, Germany
- CALPHAD XLV, May/June 2016 Awaji Island, Hyogo, Japan
- NUMIFORM 2016, July 2016, Troyes, France
- MMM 2016, October 2016, Dijon, France
- TOFA 2016, September 2016, Santos, Brazil

Fig. 2.3: Members of the SFB/Transregio 103 at the interaction week in Grainau in February 2017, including 13 ICAMS members.

Organisation of ICAMS

3. Organisation of ICAMS

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Scale Bridging Thermodynamic and Kinetic Simulation
Chair: Prof. Dr. Ingo Steinbach

Micromechanical and Macroscopic Modelling
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Chair: Prof. Dr. Jörg Neugebauer

Input Data and Validation
Lehrstuhl Werkstoffwissenschaft, RUB
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Processing and Characterization
Institut für Eisenhüttenkunde, RWTH Aachen
Chair: Prof. Dr.-Ing. Wolfgang Bleck

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>> Board of Directors

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Prof. Dr. Ingo Steinbach	Department Scale Bridging Thermodynamic and Kinetic Simulation
Dr. Rebecca Janisch	Representative of the Scientific Staff
Niklas Caesar	Representative of the Non-Scientific Staff
Arpit Mishra	Students' Representative

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Department Atomistic Modelling and Simulation AMS

4. Department Atomistic Modelling and Simulation

Prof. Dr. Ralf Drautz

Research

Within the modelling activities of the three ICAMS departments, the department Atomistic Modelling and Simulation works on the finest, most fundamental length scale of atomistic simulations. Our research has two main objectives: First, to obtain effective interatomic interactions from fundamental theories of the electronic structure and second, to employ the effective interatomic interactions in large-scale and long-time atomistic simulations and in this way obtain effective parameters that may serve as input for the modelling activities in the two other ICAMS departments. Effective interatomic interactions are obtained by systematically coarse graining the electronic structure at two levels of approximation. In a first step, the electronic structure is simplified to the tight-binding approximation by a second-order perturbation expansion of density functional theory in a minimal basis representation. Work at this level of coarse graining is carried out in close collaboration with the ASG Modelling. In a second step, bond-order potentials are derived as an analytic approximation to the exact solution of the tight-binding model. The analytic bond-order potentials are developed in close collaboration with Professor David Pettifor, University of Oxford.

The bond-order potentials are then used in large-scale and long time atomistic simulation of the structural stability and the mechanical response of a material or for analyzing the kinetics of a phase transformation. In this way a coherent link from the electronic structure to the continuum description of materials on the meso- and macroscale is obtained. As effective interatomic interactions may be derived for a wide variety of elements, interatomic potentials may be generated for transition metals and their alloys as well as semiconductors and sp-valent materials, including the effects of charge transfer and magnetism.

High-throughput density functional calculations are used to explore the chemical phase space of binary and ternary compounds and to validate trends in structural stability that are predicted by the simplified models of the electronic structure and the bond-order potentials. The high-throughput density functional simulations also help to improve and re-parameterize thermodynamic databases.

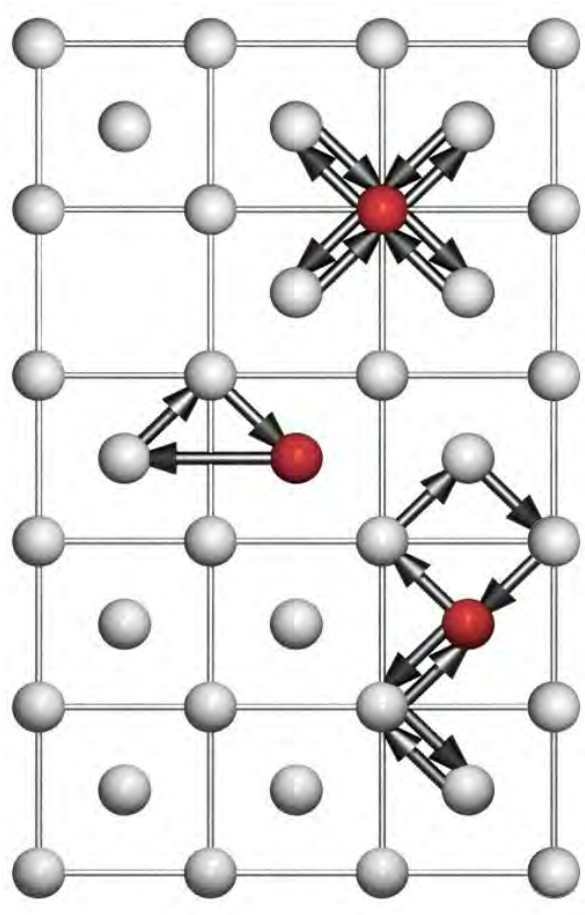


Fig.: 4.1: Within the framework of bond-order potentials the difference of the binding energy between atomic configurations is attributed to particular geometric features.

Structure

Three research groups reflect the department's aim to coherently link the different modelling hierarchies from the electronic structure through atomistic simulations to meso- and macroscopical modelling.

- Atomistic simulation of structural and phase stability (Dr. Thomas Hammerschmidt)
- Atomistic simulation of the kinetics of phase transformations (Dr. Jutta Rogal)
- Atomistic simulation of mechanical behaviour (Dr. Matous Mrovec)

In the years 2015 and 2016 8 PhD theses have been completed at AMS and 9 internal and 2 external doctoral projects are currently on-going.

AMS

4.1 Atomistic Simulation of Structural and Phase Stability

Group leader:
Dr. Thomas Hammerschmidt

Group members:
Dr. Jan-Michael Albina
Dr. Miroslav Čák
Marc Densow
Jan Jenke
Dr. Alvin Noe Ladines
Anika Marusczyk
Aparna Puchkayala Appaiah Subramanyam
Ning Wang

Introduction

The main focus of the research group Atomistic Simulation of Structural and Phase Stability is on the reliable and robust prediction of structural stability and phase stability of technologically relevant materials. In order to make direct contact with experiments, we include finite temperature, complex microstructures and multi-component chemistry.

Current topics comprise (i) precipitates of intermetallic phases, in particular topologically close-packed phases in steels and superalloys, (ii) extended defects such as planar faults and dislocations in superalloys and high-entropy alloys, (iii) magnetism at finite temperature in iron and steel and (iv) degradation of cathode materials in Li-ion batteries during dis-/charging.

These topics are addressed with a hierarchy of atomistic simulation methods that range from high-throughput density-functional theory calculations to tight-binding and analytic bond-order potentials. The research group focuses particularly on the development, implementation and application of bond-order potentials for large-scale atomistic simulations.

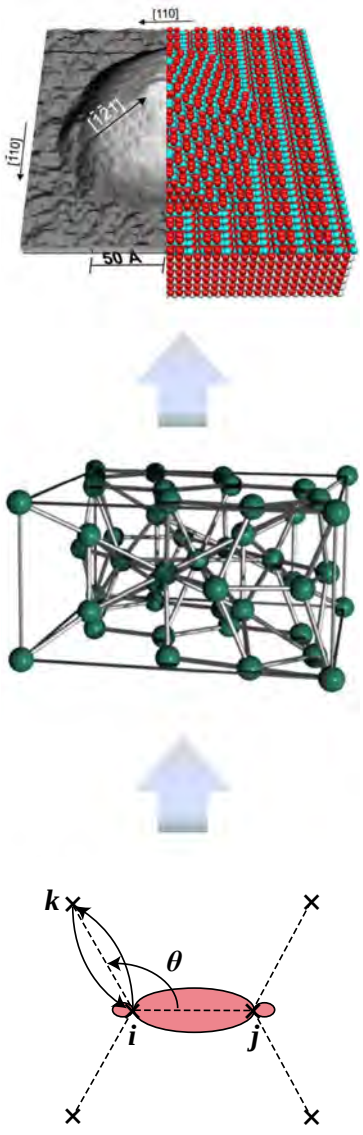


Fig.: 4.2: Coarse graining from the electronic to the atomistic modelling hierarchies. In a first step, the electronic structure is simplified to a tight-binding model. Next, using a moments expansion, the bond-order potentials are obtained. The bond-order potentials may then be used for further simulations.

The parameterization of the bond-order potentials is carried out with a semi-automatic parametrization scheme based on tight-binding models. The atomistic simulations are complemented by the development and application of structure maps. These maps chart the bonding chemistry of known compounds based on physically intuitive descriptors that enable us to predict structural stability in novel multi-component alloys.

Competences

- Analytic bond-order potentials
- Structure maps for d-d and p-d valent systems
- Automated high-throughput density-functional theory calculations
- Structural stability, point defects and interfaces of intermetallic phases (e.g. in Ni-based and Co-based superalloys)
- Magnetism at finite temperature in iron and steel

AMS

4.2 Atomistic Simulations of the Kinetics of Phase Transformations

Group leader:
Dr. Jutta Rogal

Group members:
Tanmoy Chakraborty
Dr. Grisell Díaz Leines
Alberto Ferrari
Maximilian Grabowski
Yanyan Liang
Sarath Menon
Martin Staadt

Introduction

The research group has its focus on the development and application of methods for long-time-scale atomistic simulations. The two main research areas are (i) the diffusion of impurities in the presence point and extended defects (e.g. diffusion of d-band elements in Ni-based superalloys), and (ii) the kinetics of phase transformations (e.g. formation of topologically close-packed phases, martensitic transformation in high-temperature shape memory alloys, nucleation during solidification).

Atomistic processes dominating the long-time dynamics of impurity diffusion, solid-solid phase transformations or nucleation belong to the class of so-called rare events. In this context, rare events comprise processes that require transitions between local minima of the potential energy surface that are separated by sizeable energy barriers. This leads to a separation of time scales between the short-time dynamics within each local minimum (e.g. lattice vibrations) and the long-time dynamics between the minima (e.g. diffusion, structural rearrangements), which makes it impossible to study such problems with classic molecular dynamics simulations. If the dynamics of the rare events can be described correctly based on the underlying atomistic processes, it is possible to follow the time evolution of a system over an extended time scale.

Within the group, various techniques, such as accelerated molecular dynamics, kinetic Monte Carlo, or transition path sampling are utilised to investigate rare events.

Competences

- Nucleation and phase transformation
- Diffusion
- (Adaptive) kinetic Monte Carlo
- Transition path sampling
- (Accelerated) molecular dynamics

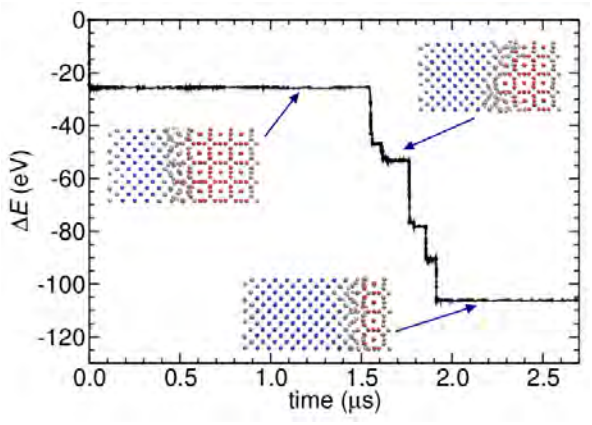


Fig.: 4.3: Change in energy along an adaptive kinetic Monte Carlo trajectory showing the transition from an A15 to a BCC structure in molybdenum. The total simulation time reaches up to microseconds at a temperature of T=300 K.

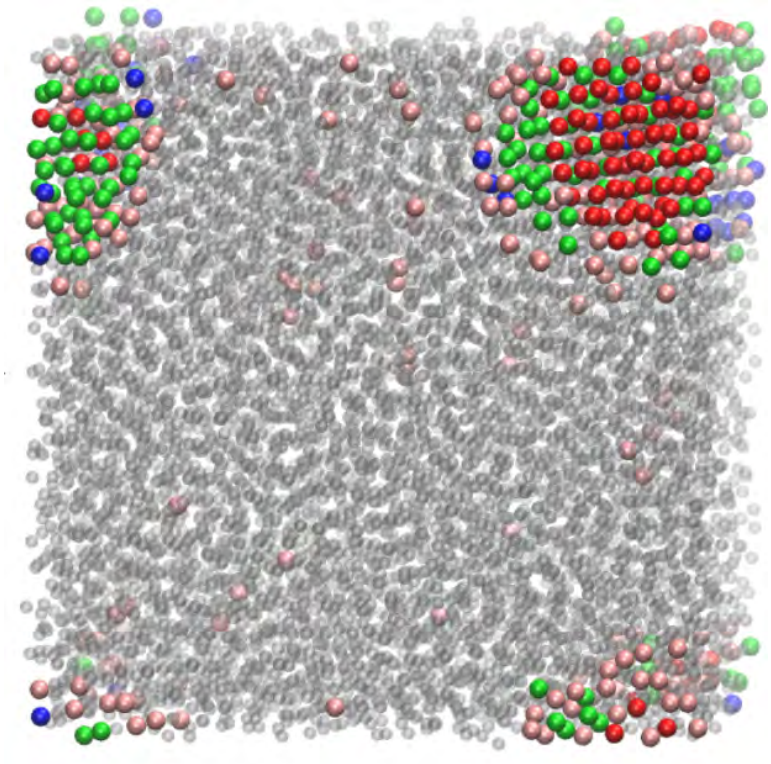


Fig.: 4.4: Growing nucleus during solidification in nickel. The snapshot was taken from a transition path sampling simulation. The different colours denote different local structures: red for FCC, green for HCP, blue for BCC, rose for pre-structured and grey-transparent for liquid.

AMS

4.3 Atomistic Simulation of Mechanical Behaviour

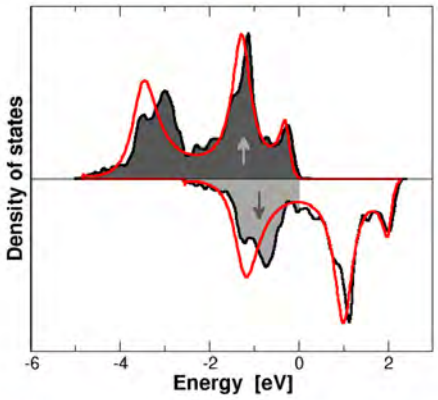
Group leader:
Dr. Matous Mrovec

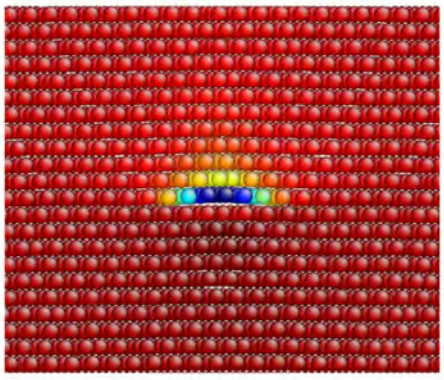
Group members:
Arpit Mishra
Malte Schröder

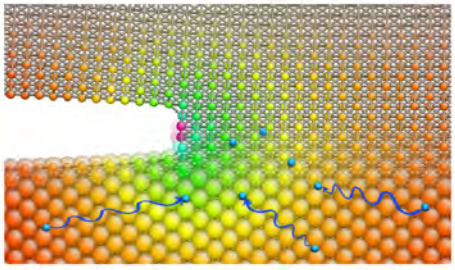
Introduction

The primary goal of the research group Atomistic Simulation of Mechanical Behaviour is to uncover the relationship between phenomena occurring on the atomic scale and macroscopic mechanical behaviour. We start with the modelling of intrinsic material properties related to chemical bonding but eventually concentrate on the role of crystal imperfections. The imperfections encompass fundamental crystal defects, such as vacancies, dislocations and grain boundaries in single-component crystalline materials as well as complex microstructural features such as semicoherent interfaces, precipitates and secondary phases that constitute the microstructure of technologically important multi-phase and multi-component systems.

The materials we are interested in include those with prototypical metallic and covalent chemical bonding and also those with mixed metallic-covalent or covalent-ionic character such as transition metals and their compounds, intermetallics, and complex alloys. The methods and models we employ span the whole atomistic modelling hierarchy from accurate first-principles methods through approximate electronic structure approaches to empirical interatomic potentials. We focus on the development and application of bond-order potentials for bridging from density functional theory to large atomistic simulations. We integrate the atomistic simulations with mesoscale techniques (DDD, kMC), phenomenological and continuum theories as well as experiments.







Competences

- Tight binding and bond-order potentials
- Transition metals and their compounds
- Crystal defects and imperfections
- Hydrogen embrittlement
- Perovskite oxides

Fig. 4.5: From electrons to atoms to mechanical properties: Electronic density of states for α-Fe from magnetic bond-order potential calculations (top), core structure of a mixed 1/2<111> dislocation in α-Fe (middle), and schematic picture of a microcrack attracting H atoms (bottom).

AMS

4.4 Simplified Models of the Electronic Structure (until August 2016)

Group leader:
Prof. Dr. Georg Madsen (now TU Wien, Austria)

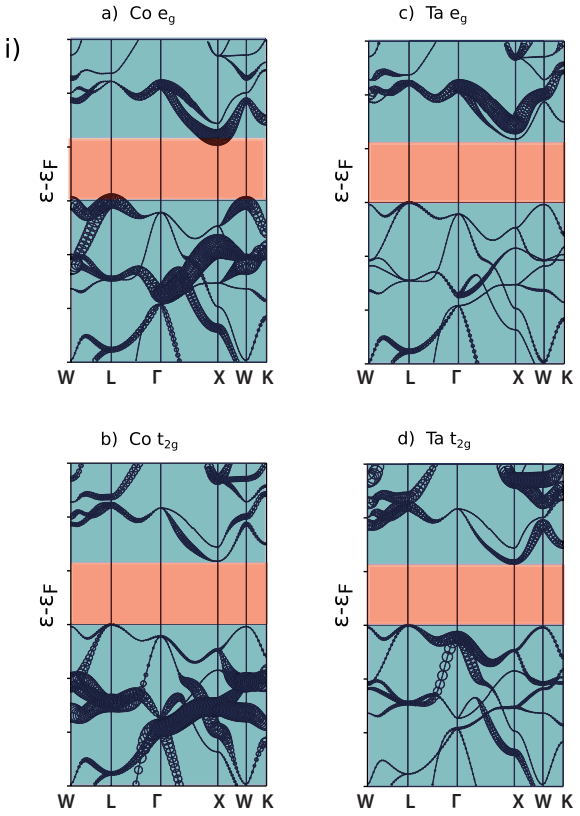
Group members:
Dr. Sandip Bhattacharya
Bonny Dongre

Introduction

Our group deals with both high-throughput materials discovery and method development. We are interested in predicting new thermoelectric materials which can be used for waste heat recovery. Furthermore, our interest lies in heat management for different material structures.

The methods used in the research group include first principles estimation of transport properties from Boltzmanns' transport equation, stability of point defects and carrier concentration, predicting stability of alloys, and quicker and more accurate first-principles estimation of thermal conductivities. We explore several materials systems, some of which are sulfides, half-Heusler, silicides (FeSi, Mg_2Si) and SnSe.

Our experimental collaborators include partners from RUB (MEMS), DLR, IMRA-SAS Europe, University of Bordeaux, and University of Stuttgart.



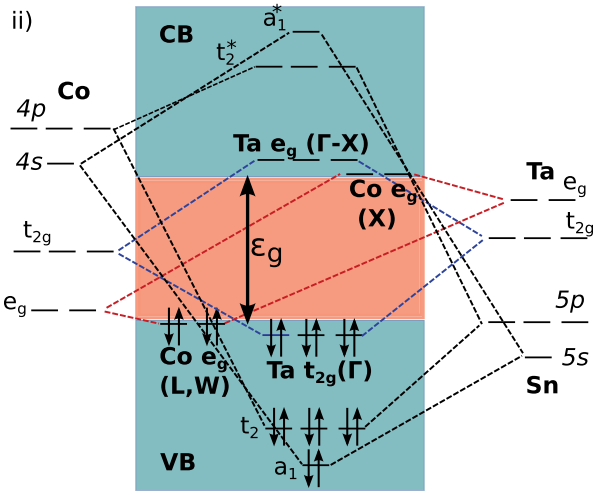


Fig. 4.6: (i) The orbital contributions to the bandstructure of TaCoSn, a new p-type half-Heusler predicted with our material design techniques [Journal of Materials Chemistry C 4, 11261-11268 (2016)] (ii) Molecular Orbital theory understanding of the half-Heusler electronic structure.

Competences

- Ab-initio estimation of thermal conductivity
- Defect thermochemistry
- High-throughput algorithms
- BoltzTrap
- ALMA-BTE for devices

Department Scale Bridging Thermodynamic and Kinetic Simulation STKS

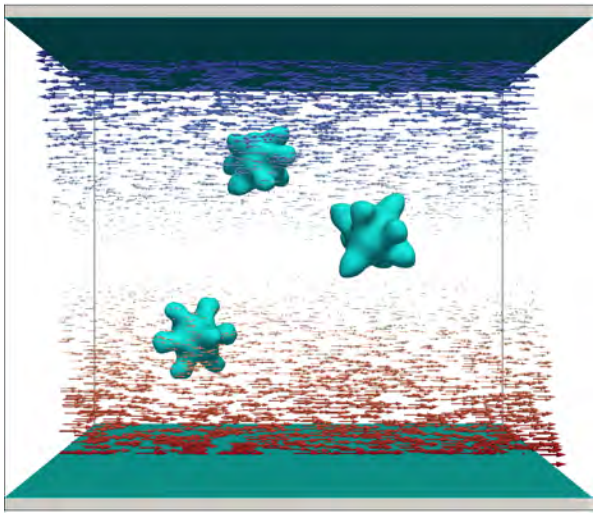
5. Department Scale Bridging Thermodynamic and Kinetic Simulation

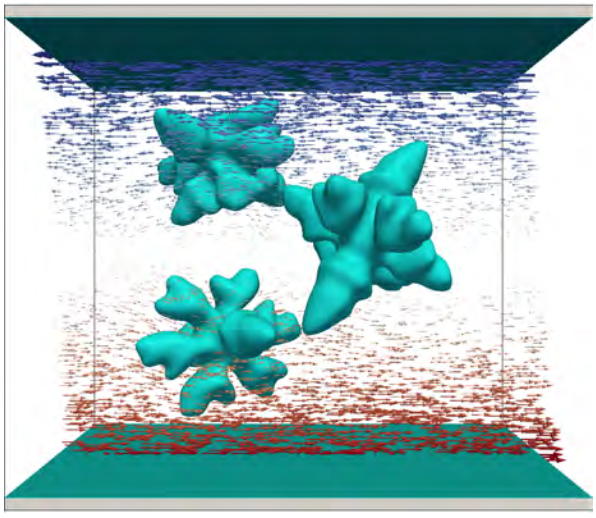
Prof. Dr. Ingo Steinbach

Research

Phase transformations are phenomena of general importance and play a significant role in all areas of materials processing. They determine the microstructure of materials and control their macroscopic properties. The research activities in the department focus on the mesoscopic scale of heterogeneous multiphase microstructures. We apply different theoretical methods to investigate the constitutive laws controlling microstructure evolution during various stages of materials processing, ranging from solidification to solid-state transformations during thermal processing.

In a scale-bridging approach we incorporate first principles calculations of phase stability and transport coefficients and analyze our results with respect to macroscopic properties of condensed matter. Among numerical techniques applied within our department are first-principles methods for phase stabilities, the CALPHAD method (CALculation of PHAse Diagrams) to calculate phase stability, the phase-field method to describe phase transformations and microstructure evolution in crystalline materials. Last, but not least, the lattice Boltzmann method is applied to solve surface tension driven flow.





Structure

The department's activities are organised in four groups focussing on different techniques and scales.

- Computational Thermodynamics/CALPHAD
  (Dr. Suzana G. Fries)
- Phase-field Simulations of Microstructures
  (Dr. Oleg Shchyglo)
- Theory and Simulation of Complex Fluids
  (PD Dr. Fathollah Varnik)
- Solid-Solid Interface Kinetics
  (Dr.-Ing. Reza Darvishi Kamachali)

5 PhD theses have been completed during the last two years and 12 internal as well as one external doctoral projects are currently on-going at STKS.

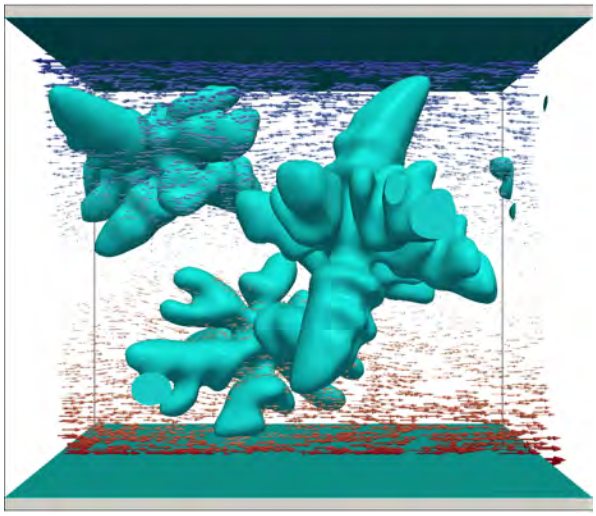


Fig. 5.1: Mg-Al dendrites in shear flow imposed as a boundary condition.

STKS

5.1 Computational Thermodynamics/CALPHAD

Group leader:
Dr. Suzana G. Fries

Group members:
Rahul Cherukuri
Irina Roslyakova

Research

The goal of the group is to incorporate first-principles calculated quantities into the thermodynamic modelling of Gibbs energies of stable and metastable phases following the CALPHAD method, in order to provide robust and sustainable multiphase thermodynamic data for microstructure simulations. The methodology to achieve this goal is developed within the Sapiens project. The use of density functional theory (DFT) to calculate electronic and vibrational contributions to heat capacity opens the possibility for a better understanding and, as a consequence, better controlling of the evolution of those contributions with temperature. This provides a physical insight into the pure mathematical parameters used in the CALPHAD Gibbs energies temperature dependence. For the composition dependence of Gibbs energies describing ordered phases, we map the configuration of several crystal structures and calculate enthalpies of formation at 0 K using DFT (in collaboration with AMS). We assume a Bragg-Williams approximation for configuration entropy as the main contribution to the entropy. For the disordered phases we have given preference to the EMPO-CPA method, but SQS and the cluster expansion method are also under investigation. The

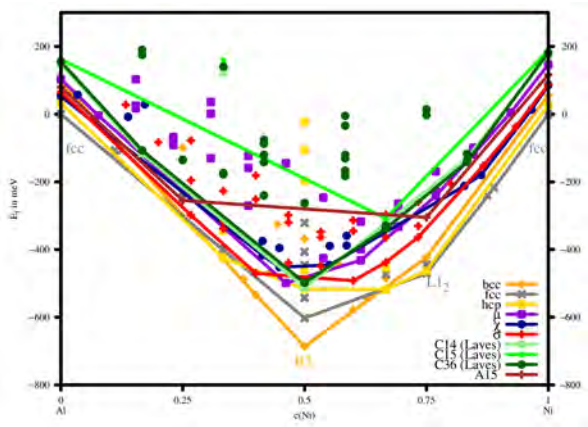


Fig. 5.2: Enthalpies of formation for all stable (and metastable) phases in the Ni-Al systems calculated by DFT at 0 K .

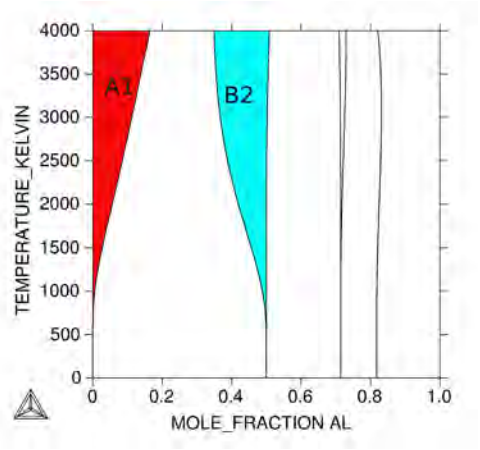


Fig. 5.3: Calculated Ni-Al phase diagram using the DFT results for the configuration enthalpies and the Bragg-Williams-Gorsky (BWG) approximation for configurational entropic contribution.

application of our Gibbs energies functions database to multicomponent, multiphase materials requires a realistic description of experimentally observable quantities. In order to fulfil this requirement, we construct an extensive experimental database which is used for training the physical parameter of the models. We do add excess quantities when necessary, but with our method they are usually only a small correction to the well-controlled physical quantities. Proprietary thermodynamics databases for technical alloys are improved using these corrections.

Competences

- Thermodynamic modelling
- Order-disorder solid solutions
- Open Calphad library development
- Critical evaluation of experimental input data

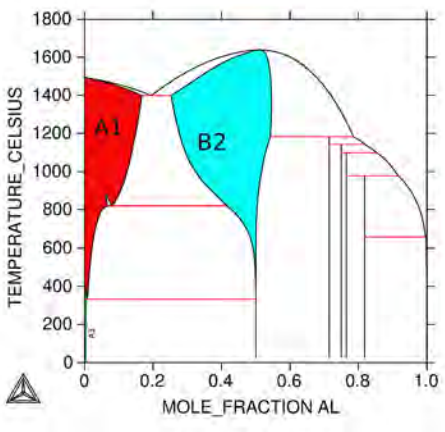


Fig. 5.4: Ni-Al phase diagram calculated using the TCNI8 proprietary thermodynamic database based on the CALPHAD method.

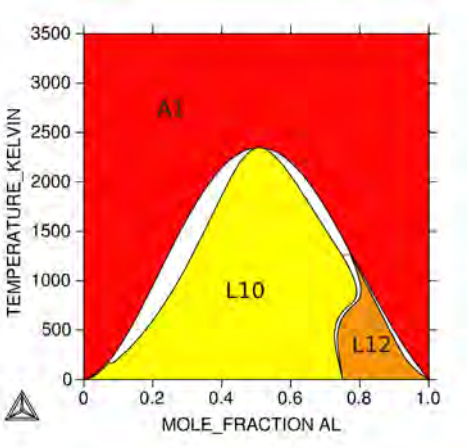


Fig. 5.5: The Ni-Al FCC based metastable phase-diagram calculated using the DFT-BWG approximation only.

STKS

5.2 Phase-Field Simulations of Microstructures

Group leader:
Dr. Oleg Shchyglo

Group members:
Katrin Abrahams
Muhammad Adil Ali
Dr. Guanxing Du
Johannes Görler
Stefan Hubig
Dr.-Ing. Alexander Monas
Seyed Mohammad Mehdi Noori
Raphael Schiedung
Matthias Stratmann

Introduction

The research group focuses on the development of new methods for phase-field simulations of microstructures in complex materials. At present, the range of applications for phase-field modelling includes solidification, grain growth, eutectic and peritectic reactions, recrystallization, and martensitic transformations. To make quantitative predictions of the microstructure formation in these processes by using the phase-field method, it is important to start from the reliable free energy functional. This requires access to the free energy contributions related to chemical composition, elasticity parameters and plastic laws for the materials under study. While the composition-temperature dependence of the free energy is widely available in databases, the free energy contribution from elasticity and plasticity data is not easily available. Our goal is not only to provide the reliable simulation platform for the phase-field simulations, but also to provide the free energy contributions which are at present omitted in the thermodynamic databases. In collaboration with the Computational Thermodynamics/CALPHAD group, we develop the free energy model, which incorporates not only the chemical degrees of freedom but also include the stress dependence of the free energy. Such a free energy functional is a key ingredient for the study of the bainite and martensite formations in steel which are among our primary objectives.

Competences

- Phase-field modelling
- Phase transformations
- Microscopic elasticity theory
- OpenPhase library development

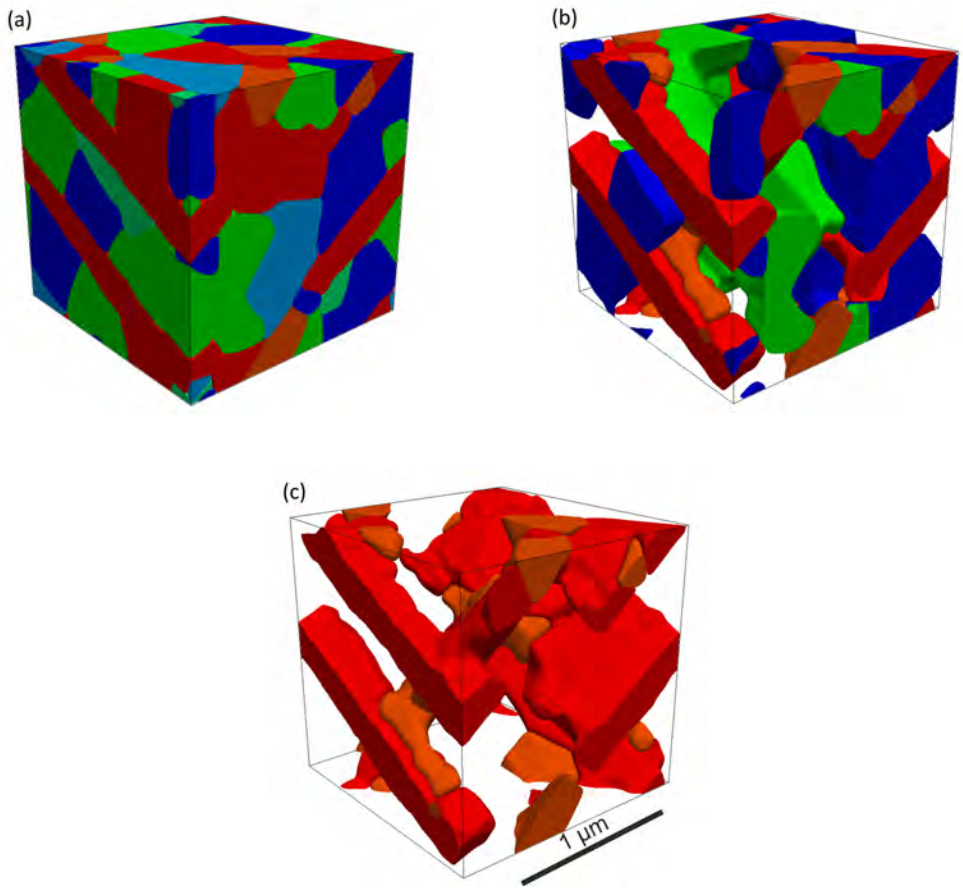


Fig. 5.6: Simulated martensite microstructure of carbon steel: (a) complete martensite microstructure (b) single martensite packet and (c) martensite blocks.

STKS

5.3 Theory and Simulation of Complex Fluids

Group leader:
Apl. Prof. Dr. habil. Fathollah Varnik

Group members:
Muhammad Reza Hassani
Elias Mahmoudinezhad Zirdehi
Amol Subhedar
Samad Vakili

Introduction

The main research focus of the group is on transport phenomena and phase transformations in fluidic media.

Problems addressed by the group include a variety of physical phenomena such as wetting and capillarity, rheology and shear-induced diffusion in dense suspensions of deformable particles (such as red blood cells and vesicles), deformation and response in highly viscous amorphous materials and chemo-mechanical coupling in shape memory polymers.

On the methodological side, the group uses molecular dynamics (MD) simulations, the lattice Boltzmann method (LBM) as well as hybrid approaches combining the LBM for fluid flow either with MD for particle dynamics in the flow or with finite element method (FEM) to study suspension rheology of deformable closed membranes as a model for red blood cells and vesicles.
Recently, the complex fluids group commenced to combine the phase-field (PF) method for phase transformation kinetics and microstructure evolution with the lattice Boltzmann method in order to account for the effect of transport by the flow on the interface dynamics during solidification. This approach has been further extended by introducing wetting and capillarity into the coupled PF-LBM scheme and is used to investigate effects of capillarity-induced grain rearrangements on the microstructure in liquid phase sintering.

During the past five years, the group has also made major contributions to the methodological development within the lattice Boltzmann framework. By introducing thermal fluctuations within the so-called non-ideal fluid lattice Boltzmann methods, the LBM has been advanced to the stage of addressing wetting phenomena on the nano-scale.

Competences

- Lattice Boltzmann modelling
- Supercooled liquids and glasses
- Suspension rheology
- Molecular dynamics of polymers
- Phase field lattice Boltzmann coupling

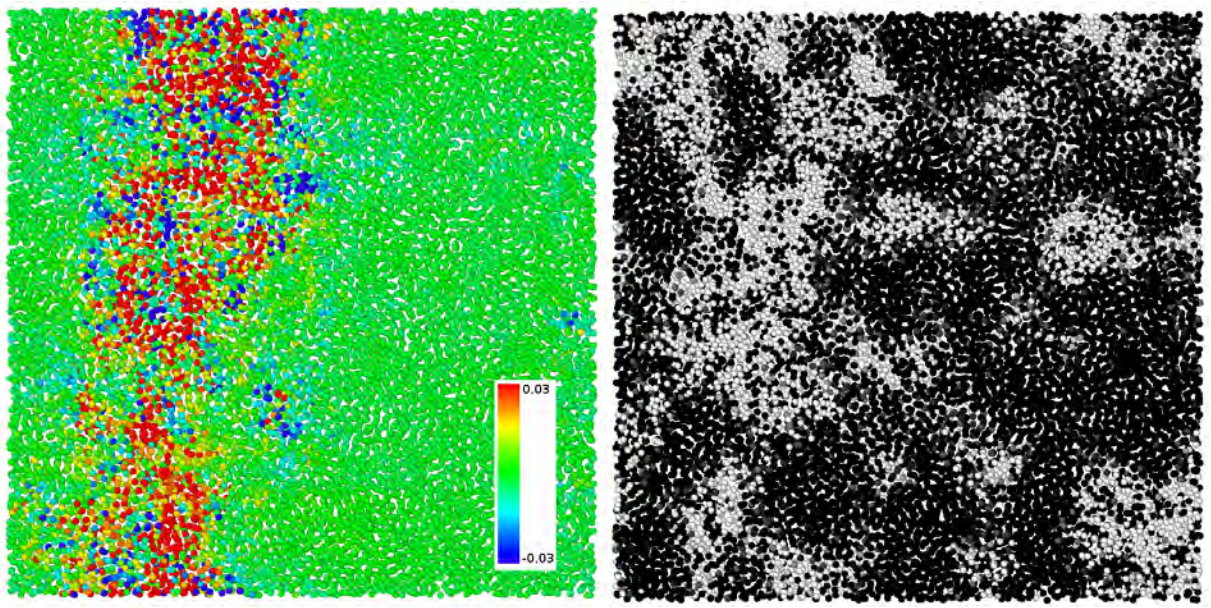


Fig. 5.7: Molecular dynamics simulation results on shear band formation in a model metallic glass (a binary Lennard-Jones alloy). (a) Colour coded shear strain within a plane passing through the center of the sample. The colour scheme shows the numerical value of the strain. (b) The distribution of a non-local measure of the excess volume obtained from Voronoi-tessellation. Here, each data point gives the correlation between the excess volume of a particle and its nearest neighbours. Simulations performed by Muhammad R. Hassani using LAMMPS.

STKS

5.4 Solid-Solid Interface Kinetics

Group leader:
Dr.-Ing. Reza Darvishi Kamachali

Group members:
Muhammad Umer Bilal
Christian Schwarze

Introduction

In the group of Solid-Solid Interface Kinetics, multi-physics problems concerning interface phenomena in solid state materials are solved.

We analyse kinetic and thermodynamic theories of interface in the presence of diffusion, elastic and plastic activities based on which the development of mesoscale phase-field models and simulations are promoted. These methods are employed to discover the underlying mechanisms of the microstructure evolution in a range of nano- to microscales.

On the collective level, parallel computation and mean-field concepts are applied to link microscopic characteristics of the microstructures and their macroscopic properties. Analytical and numerical investigations are made concerning various topics including origin of grain growth, vacancy drag of grain boundaries, secondary-phase particle pinning, recrystallization, precipitation and ripening within polycrystalline materials.

A new focus on precipitation-hardened Al alloys is developing within our group with an emphasis on the fundamental aspects of precipitation and ripening under strong chemo-mechanical coupling. Recently, a new mechanism of inverse ripening of coherent precipitates and the emergence of new patterns of elastic anisotropy in the matrix have been discovered in Al alloys. We are involved in the priority program SPP 1713 *Strong coupling of thermo-chemical and thermo-mechanical states in applied materials*, leading project DA1655/1-1.

Competences

- Theories of interface kinetics
- Phase-field simulations
- Mean-field theory
- Irreversible thermodynamics

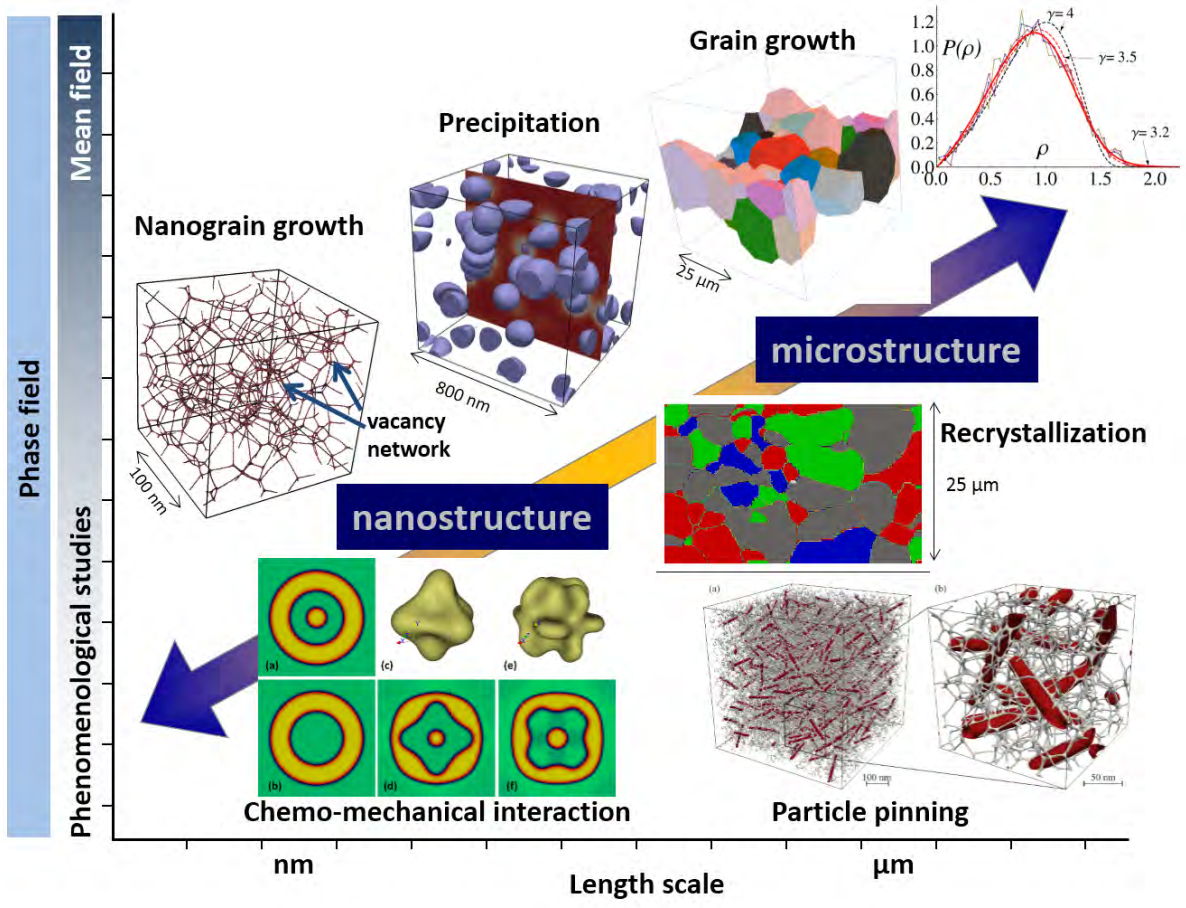


Fig. 5.8: Scales and approaches of research in the Solid-Solid Interface Kinetic group.

Department Micromechanical and Macroscopic Modelling MMM

6. Department Micromechanical and Macroscopic Modelling

Prof. Dr. Alexander Hartmaier

Research

Developing innovative materials which meet the complex requirements of a diverse range of applications is only possible if the relation between their inner structure, i.e. the microstructure, and their properties is thoroughly understood. We aim at deriving such microstructure property relationships in order to predict macroscopic mechanical properties of materials, like strength, hardness, and toughness, by employing the methods of computational materials science and multiscale modelling. To accomplish this, we typically start from macroscopic models that describe an engineering application or test (*Fig. 6.1*). At the critical spots of this macromodel, where the conditions are particularly severe and potentially damaging, a micromechanical model is employed which explicitly takes into account the local microstructure and loading conditions.

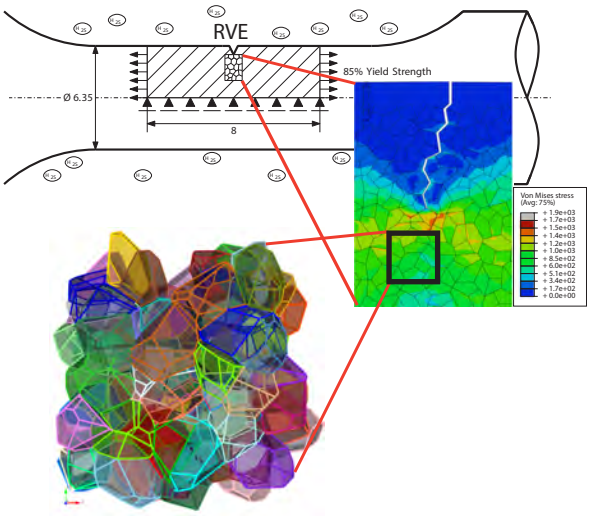


Fig. 6.1: Top-down scalebridging approach demonstrated for a NACE-A test specimen in a sour environment under a mechanical load of 85% of its yield strength. Where the corrosive attack creates microcracks at the surface, a micromechanical model (RVE) is considered.

The microstructure in such micromechanical models is described by representative volume elements (RVES) which can be developed on different purpose-specific levels of detail to represent either phases as homogeneous regions or individual grains within phases or even sub-structures within grains (*Fig. 6.2*). Such micromechanical models mainly serve two purposes: (i) they provide insight into the critical deformation and failure mechanisms and how they depend on the microstructure and local thermal, mechanical, and chemical conditions of the material; (ii) they serve as the basis for the macroscopic descriptions of materials properties in form of flow rules as they are used in continuum plasticity. This latter step of developing macroscopic flow rules based on micromechanical models is termed homogenization and can be used to take microstructural properties and mechanisms implicitly into account in macroscopic models of engineering problems.

In some situations, it is necessary to refine microstructural descriptions even to the level of individual (discrete) dislocations and their interactions with the microstructure. Such discrete dislocation dynamics (DDD) models are, for example, employed to study the deformation and creep behaviour of single crystal superalloys within the DFG-funded Collaborative Research Centre SFB/TR 103 *Superalloy*

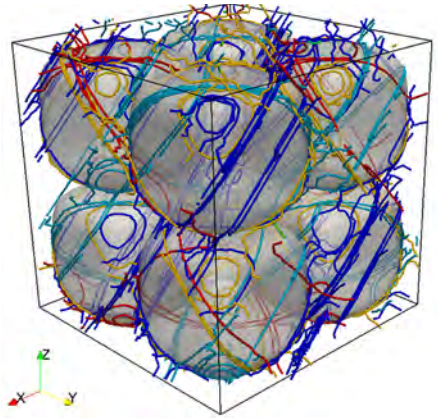


Fig. 6.2: Discrete dislocation dynamics model of deformation and creep of a superalloy, where dislocation motion typically takes place in the channels between cuboidal γ' precipitates (S. Gao, 2016)

Single Crystals (*Fig. 6.2*). Finally, processes at interfaces such as interface sliding or cracking can only be understood on the atomic scale. Hence, such atomistic models of interfacial properties must be analysed closely (*Fig. 6.3*), and their results need to be homogenized in order to be applicable in cohesive zone models or other fracture and damage models which can be applied on the macroscale.

As described above, predicting materials behaviour in a quantitative sense requires the a priori knowledge of the microstructure and also of the properties of all phases, their interfaces, and grain boundaries. The development of methods for obtaining a proper characterization of realistic microstructures and local materials properties is one vital focus of research in our department. In some cases, the dynamical evolution of microstructures during deformation needs to be taken into account explicitly. In a joint research effort with the ICAMS department Scalebridging Thermodynamic and Kinetic Simulation (STKS), advanced crystal plasticity models which take into account dislocation density evolutions are combined with the phase-field code OpenPhase developed in the department STKS.

The department MMM is organized into three research groups, namely 'Mechanical Properties of Interfaces' (Rebecca Janisch), 'Micromechanics of Large Deformations' (Napat Vajragupta), and 'Discrete Micromechanics and Fracture' (Hamad ul Hassan). The group leaders of the latter two groups joined ICAMS in 2016 and strengthen our team by continuously advancing our modelling capabilities in their fields. In the years 2015 and 2016 9 PhD theses have been completed at MMM and currently, 4 internal and 4 external doctorate projects are underway, the latter at industrial partners of ICAMS.

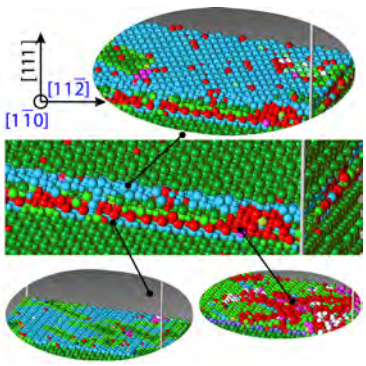


Fig. 6.3: Atomistic description of interfacial deformation processes in intermetallic TiAl phases (M. Kanani, 2016).

MMM

6.1 Mechanical Properties of Interfaces

Group leader:
Dr. Rebecca Janisch

Group members:
Abril Azocar Guzman
Xiang Huang
Ankit Izardar
Tapaswani Pradhan
Zhangqi Wang

Introduction

The research group Mechanical Properties of Interfaces carries out atomistic simulations to understand the fundamental processes that occur at interfaces under different loading conditions and which determine the strength and deformability of polycrystalline microstructures in metals and alloys. Based on this understanding, predictive physical models are established that connect the atomistic details of individual grain boundaries, such as structural units and chemical composition, to the effective interface behaviour. Such models can be used in mesoscale simulations of microstructure evolution, deformation, and fracture to identify microstructures with optimised mechanical properties.

Recent work focused on the effect of alloying elements, vacancies, and strain on the deformability and strength of ferritic steel, as well as on the effect of strain and interface structure on the deformation mechanisms in aluminium and titanium-aluminium alloys. In both cases it was possible to connect fundamental physical and structural properties to the mesoscopic behaviour either observed experimentally or in molecular dynamics simulations. For instance, the dynamical shear behaviour of grain boundaries in face-centred cubic Al, as well as in γ-TiAl, revealed several deformation mechanisms which can be understood based on a multi-layer analysis of the stacking fault energies in the grain boundary and adjacent planes. This allows the formulation of an energy-based model of shear that can in turn be used for ab-initio based alloy design.

Competences

- Ab initio electronic structure calculations
- Molecular dynamics simulations
- Interface mechanics and thermodynamics

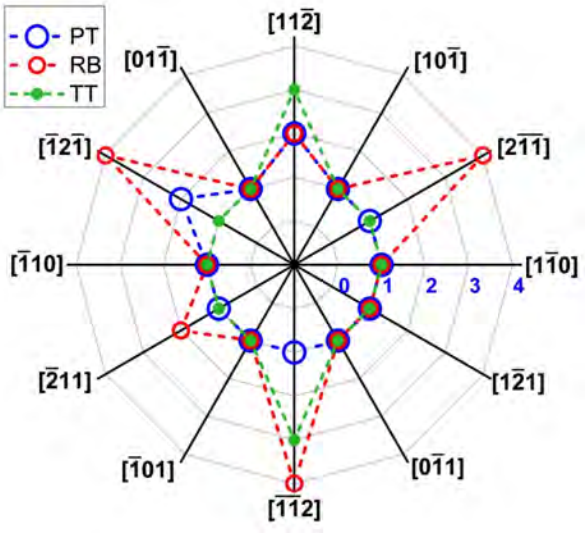


Fig. 6.4: Sliding mechanisms for three different rotational boundaries in TiAl for twelve different directions. PT: pseudo-twin boundary, RB: rotational boundary, TT: true twin boundary. The distance from the origin represents the mechanism: 1: rigid grain sliding, 2: twin nucleation and growth, 3: grain boundary migration, 4: in-plane dislocation nucleation in several layers.

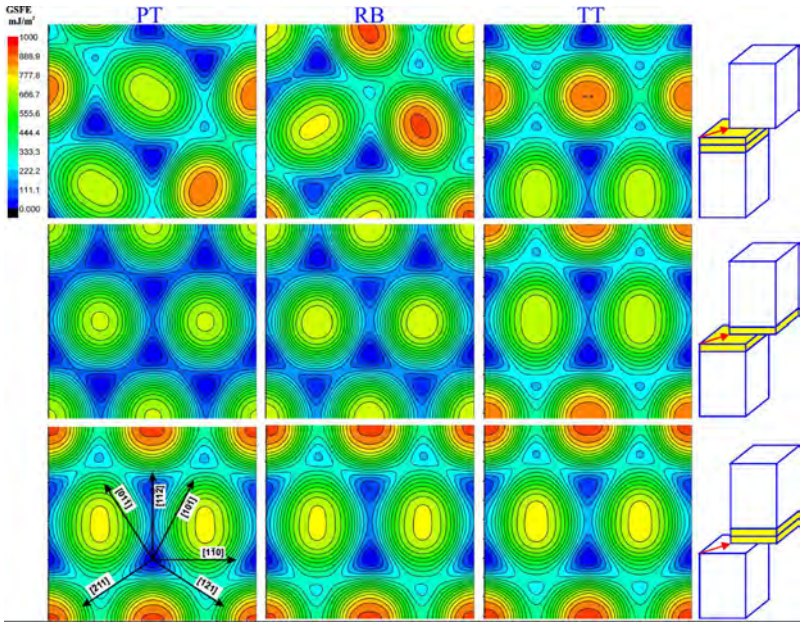


Fig. 6.5: Multilayer generalized stacking fault energy surface for the pseudo-twin boundary in TiAl. The energy landscape for the onset of a shear instability is shown for the grain boundary layer (middle layer) as well as for the crystallographic planes below and above. An evaluation of all three layers enables prediction of the effective mimimum energy path and the deformation mechanism along specific directions.

MMM

6.2 Crystal Plasticity Modelling and Simulation (until October 2016)

Group leader:
Dr.-Ing. Anxin Ma

Group members:
Dr.-Ing. Siwen Gao
Rehman Hameed
Muralikiran Krishnakumar

Introduction

This research group focuses on deformation modelling of important engineering materials, such as transformation induced plasticity (TRIP), assisted steels and nickel-based superalloys. In many cases, a representative volume element (RVE) with proper homogenization is constructed for one material point. Sometimes important deformation mechanisms, e.g. non-Schmid law, and model parameters, e.g. dislocation density, are studied by discrete dislocation dynamics (DDD) and molecular dynamics (MD).

Therefore, Anxin Ma's research group works to overcome the following challenges: 1) to develop crystal plasticity models which consider multi-deformation mechanisms such as slip, twin, phase transformation and vacancy diffusion at high temperature; 2) to study additional isotropic and kinematic hardening of plastic strain gradients caused by grain boundaries and precipitates; 3) to deal with damage and micro-crack; 4) to investigate materials properties under monotonic loadings and cyclic loadings; and 5) to develop simulation tools inside the finite element method (FEM), fast Fourier transformation (FFT) and smoothed particle hydrodynamics (SPH) frameworks.

Competences

- Multi-physics type crystal plasticity
- 3D-dislocation dynamics
- Cohesive zone model
- Abaqus UMAT and UEL
- CP-FEM, CP-FFT, CP-SPH

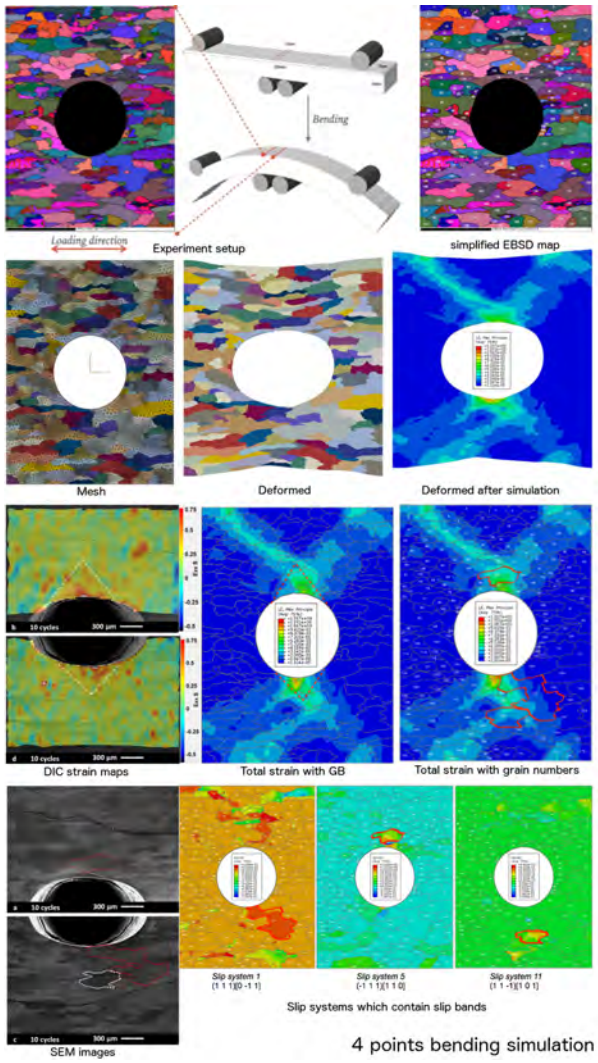


Fig. 6.6: CP-FEM simulation and experiment of an aluminium polycrystal beam with a hole under cyclic bending load. The micro-cracks initialized in deformation localization zone. There is a clear hint that the accumulated plastic shear on slip systems determines microcrack initialization. This is a joint research project of ICAMS and Warwick University (UK).

MMM

6.3 Micromechanics of Large Deformations (since May 2016)

Group leader:
Dr.-Ing. Napat Vajragupta

Group members:
Shabaz Ahmed
Waseem Amin
Daysi Gonzalez Dacasa
Jenni Engels
Dr.-Ing. Siwen Gao
Soheil Rooein

Introduction

The research group Micromechanics of Large Deformations aims at using the micromechanical modelling approach to describe large deformations of materials or components on the macroscopic scale. To achieve this goal, we focus on several key research areas including methods to generate representative volume elements (RVEs), crystal plasticity models, and homogenization or optimization schemes.

At the center of the micromechanical modelling approach, the method for generating RVEs is of crucial importance, as it must be able to quantitatively capture all the important microstructural features such as grain size and shape distributions. Hence, different platforms to construct RVEs have been developed and investigated within our research group. Our aim is to generate sophisticated microstructure models from a small number of input parameters.

As new materials with complex microstructures are constantly being developed and introduced into technology, more complicated deformation mechanisms are to be expected and will require more advanced models to describe them. Thus, we continuously intensify our expertise in crystal plasticity to consider multi-deformation mechanisms such as slip, twinning, phase transformations, and diffusional creep. In addition, the parameterization of the materials models is within the scope of our work as well.

The combination of methods for RVE generation and material modelling allows us to develop micromechanical models with which the fundamental deformation mechanisms and their dependence on microstructural features can be investigated. Furthermore, by using sophisticated homogenization techniques, the results of the micromechanical models serve as a basis for materials descriptions with advanced continuum plasticity flow rules.

Competences

- Construction of representative volume elements from quantitative description of microstructure morphology
- Crystal plasticity models and parameterization of the materials models
- Homogenization and optimization techniques to bridge microscopic-scale simulations with advanced continuum plasticity flow rules

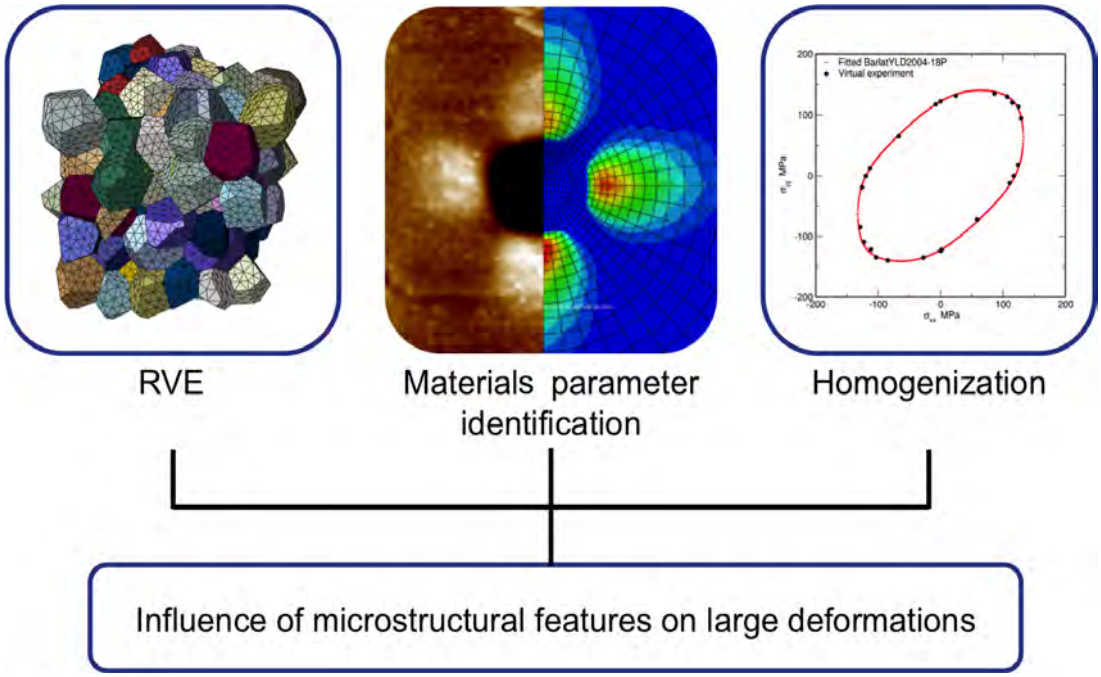


Fig. 6.7: Micromechanical modelling strategy to bridge the influence of microstructural features on large deformations.

MMM

6.4 Discrete Micromechanics and Fracture

Group leader:
Dr.-Ing. Hamad ul Hassan

Group members:
Kishan Govind
Denise Reimann
Hafiz Muhammad Sajjad
Muhammad Ibrar Saleh
Sushanth Varada
Wenye Ye

Introduction

The multi-disciplinary research of the Discrete Micromechanics and Fracture group focuses on advanced engineering materials and their response to various types of external loading and environmental conditions. The main aim of the group is the development of advanced numerical methods and their application to describe deformation and failure processes on the microstructural scale (*Fig. 6.8*).

Experimental tools are used to generate reliable input data and to validate the numerical methods.

Our analysis of localized deformation, evolution of damage as well as failure initiation and development allows the prediction of the properties, performance, behaviour under loading, and structural integrity of modern materials

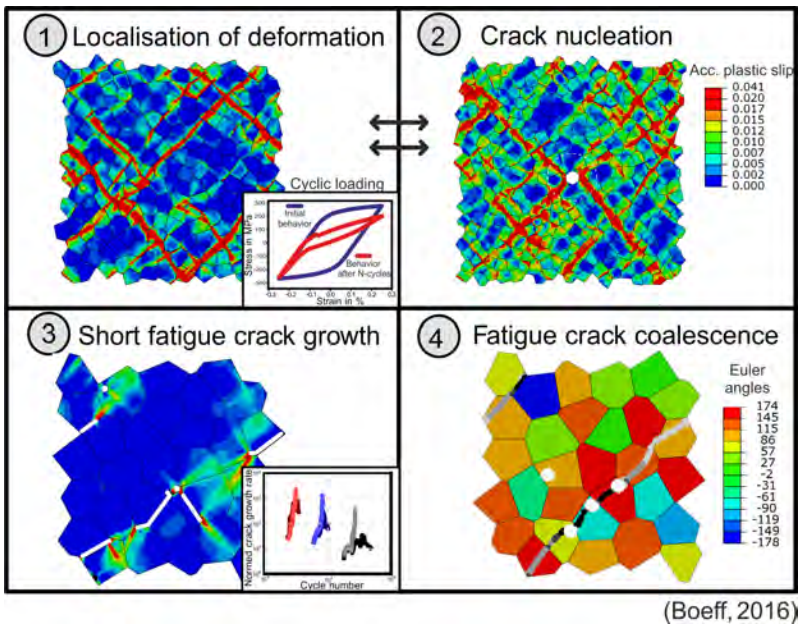


Fig. 6.8: Numerical simulation of fatigue behaviour using the Crystal Plasticity-Finite Element Method (CP-FEM). (1) Localization of deformation under cyclic loading, (2) crack nucleation due to accumulation of plastic slip, (3) short fatigue cracks grow individually, (4) coalescence of several cracks through multiple grains.

and components made from them. A major emphasis is put on the understanding of how the internal microstructure of an engineering material influences its response under application in the field. Investigations are carried out based on micromechanical principles using Crystal Plasticity-Finite Element Method (CP-FEM) to describe plasticity, fracture, damage and fatigue behaviour. The influence of a hydrogen environment on the fracture behaviour of materials is also investigated (*Fig. 6.9*). The materials we are currently working with are steels and alloys, aluminium and composites.

The research in this group is strongly interlinked with other research activities at ICAMS concerned with modelling of microstructures and the atomistic description of fracture.

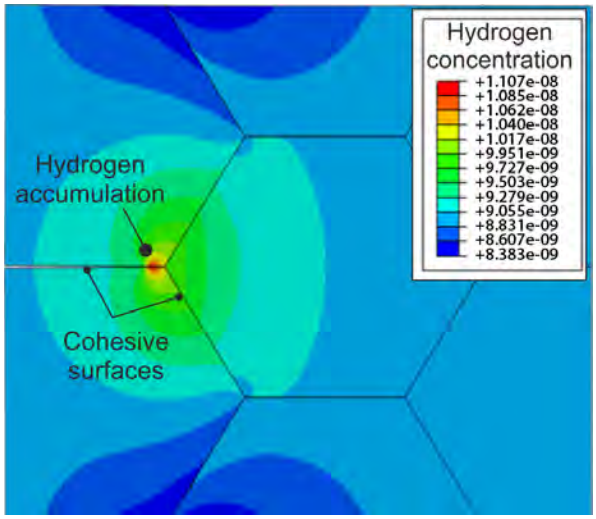


Fig.6.9: Simulation of hydrogen assisted fracture.

Competences

- Finite element modelling
- Material chraracterization and modelling
- Damage and fatigue analysis
- Micromechanical simulation of fracture
- Cohesive zone modelling and hydrogen embrittlement

High Performance Computing in Materials Science HPC

7. High Performance Computing in Materials Science

Dr. Godehard Sutmann

Group members:
Dr. Carlos Teijeiro Barjas
Hariprasath Ganesan
Marvin Tegeler

The research group High Performance Computing in Materials Science at ICAMS is working on the development of parallel methods and algorithms for the efficient simulation of materials science applications on different levels of approximation. Apart from its distinct research, the group has strong links to all ICAMS departments and supports the development of simulation codes and efficient parallelization of programs developed at ICAMS. The group follows two different directions: support of local simulation activities and research on parallel algorithms for complex simulations in materials science. Thematically, particle methods, e.g. molecular dynamics (MD) methods, have been a focus of the group, but activities also lean towards parallel phase field simulations, which support activities on the development of the *OpenPhase* software at ICAMS.

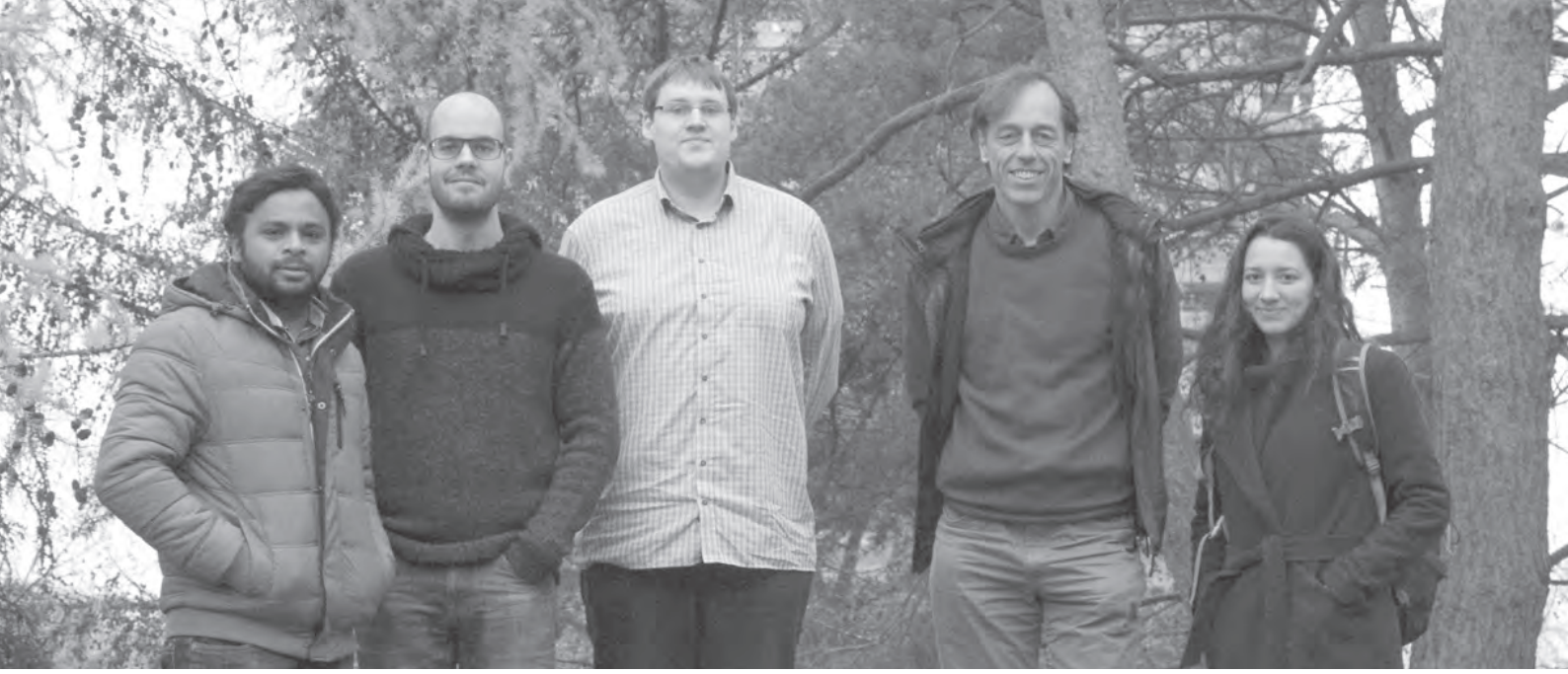
As larger or more complex simulation tasks require efficient implementations of software solutions, a main focus is the exploration of parallel techniques to accelerate existing software or to design new solutions for parallel architectures. For a number of problems, domain decomposition is a promising direction for parallelization, as it is based on a distribution of work, spent in different parts of the physical space, which is distributed onto the compute resources. If the work is homogeneously distributed over the physical space, traditional techniques, based on equal subdivisions of space, show a promising performance. But in case of time-dependent or inhomogeneous work distribution, efficiency decreases, resulting in a bad usage of computational resources.

Therefore, load balancing techniques are developed and implemented which allow for a better usage of resources and a reduction of computational cost. For mesh-based simulation techniques, e.g. finite difference methods for solving partial differential equations, block decomposition schemes were developed to distribute work between processors, based on a graph partitioning algorithm that considers the work and the communication overhead between processors.

For particle based simulations, a method based on shape transformations of domains leading to non-orthogonal regions has been developed. These techniques can be applied if a large problem is distributed onto a number of compute cores.

A suitable case is the segregation of interstitial atoms in a solid where the diffusion of C-atoms is determined by a high activation energy, and the process can be treated as a rare event on the atomistic level. To simulate such processes, a parallel hybrid Monte Carlo / molecular dynamics method has been developed, based on a manager-worker parallel algorithm, where speculative execution of tasks is explored to gain a speed-up with respect to a serial execution.

This approach proves to be successful in simulating segregation events which can only be observed in extremely long simulation runs when applying time stepping methods.



A theoretical stochastic model has been developed which was able to characterize the behaviour of the speculative execution model and shows satisfactory scaling properties for a parallel Monte Carlo scheme.

To account for multi-core architectures with shared memory parallelism, the parallelization of the bond-order potential code *BOPfox* has been extended to a hybrid *MPI/OpenMP* version. This allows using the full memory of a

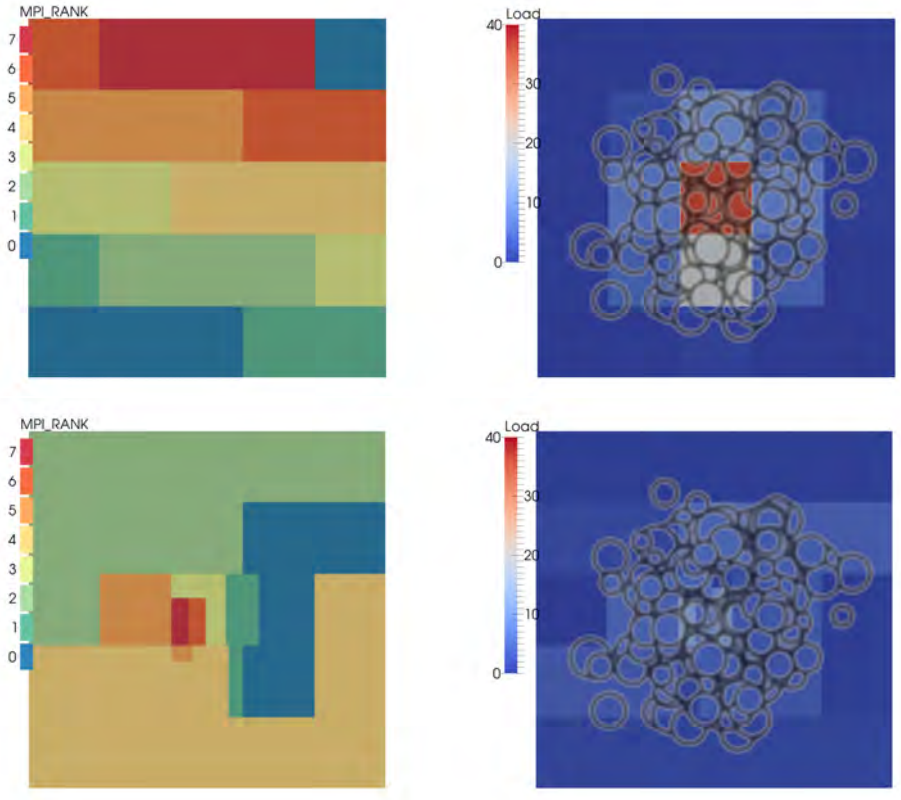


Fig. 7.1: Comparison of a parallel simulation with OpenPhase *using a domain decomposition without (top) and with (bottom) load balancing, based on a block decomposition. Left: distribution of processors; Right: colour coding for work distribution.*

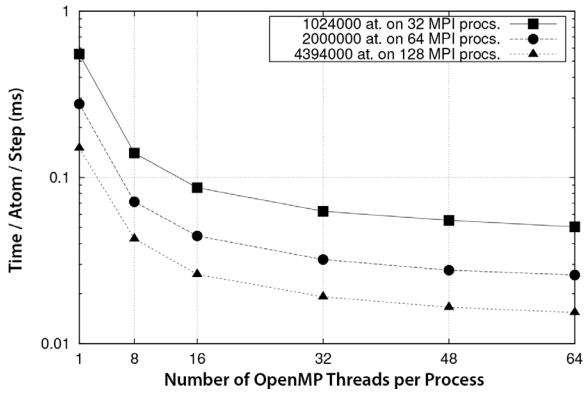


Fig. 7.2: Scaling behaviour of the parallel BOPfox *simulation code on a* IBM BlueGene/Q *for the hybrid* MPI/OpenMP *version for various problem sizes. Curves were shifted by a constant factor.*

computational node. This is often essential to satisfy the large memory requirements of bond-order computations and to parallelize the time-consuming on-node path computations within a shared memory parallelization model. The successful implementation of the parallel path computations yields a very high parallel efficiency for these by far most expensive parts of the bond-order simulations. The new implementation has been tested on the large-scale facility *JUQUEEN*, an *IBM BlueGene/Q* computer with 16 GByte memory per node, which makes it very difficult to run BOPfox with one MPI process per core (i.e. 1 GByte per core) with a traditional domain decomposition scheme. The new hybrid parallelization can be run with one MPI process per node plus an additional shared memory parallelization, where up to 64 threads can be used efficiently in the symmetric multiprocessing (SMP) mode.

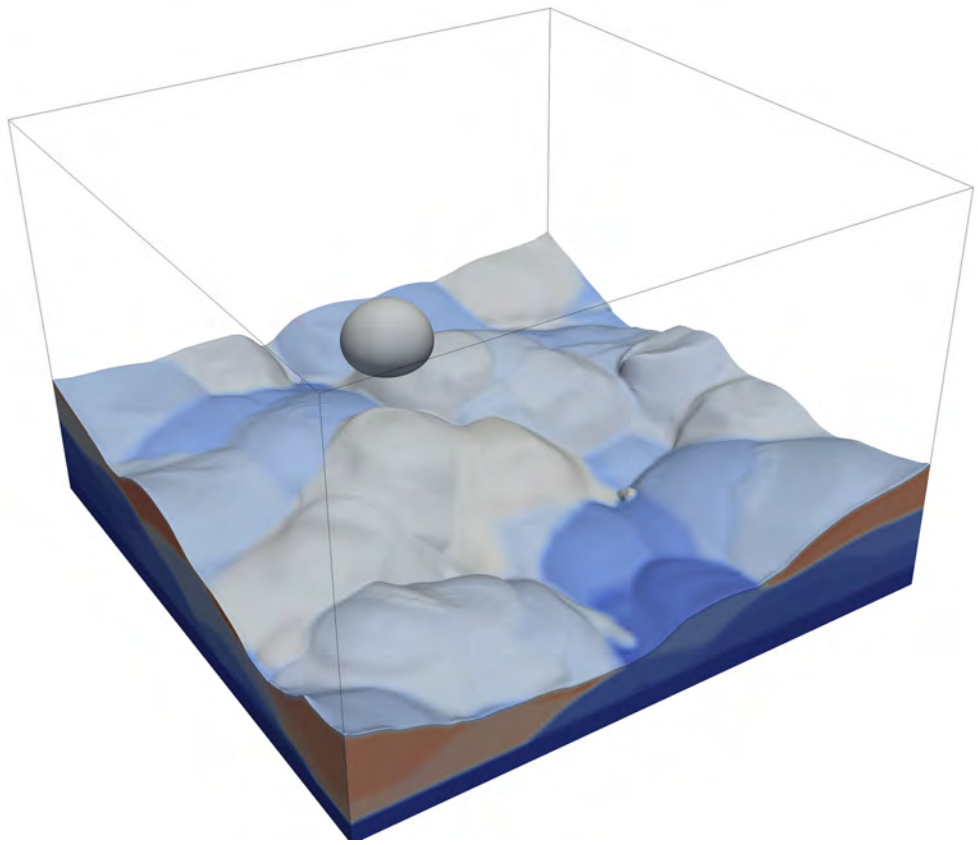


Fig. 7.3: Simulation of surface coating by particle spraying, simulated with OpenPhase.

The load-balancing of the parallel phase field simulation code *OpenPhase* was optimized. The underlying graph partitioner was compared to other partitioning schemes, showing comparable or even better performance characteristics.

As a highly demanding parallel application, a model for the structure formation in spraying processes was considered. For the case of thermal barrier coatings, a coupling between a flow field, carrying particles, and the phase-field computations has been achieved and implemented in *OpenPhase*, resulting in a high demand for balancing the load between processors. In these simulations, droplets of coating material were transported according to the surrounding gas flow, cooled down and solidified at the substrate. *Fig. 7.3* shows a complex structure formation of surface texture generated by this model.

Competences

- Parallel algorithms
- Molecular dynamics, Monte Carlo
- Particle simulation methods
- Load balancing

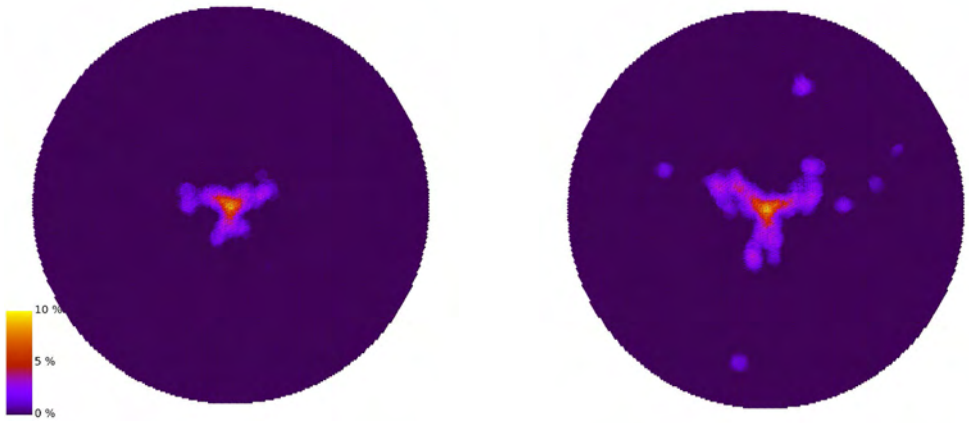


Fig. 7.4: Density distribution of carbon atoms around a screw dislocation for 0.01 wt% (left) and 0.02 wt% (right), simulated with a parallel hybrid Monte Carlo / molecular dynamics method.

Advanced Study Group Modelling

8. Advanced Study Group Modelling

Prof. Dr. Jörg Neugebauer
Dr. Tilmann Hickel

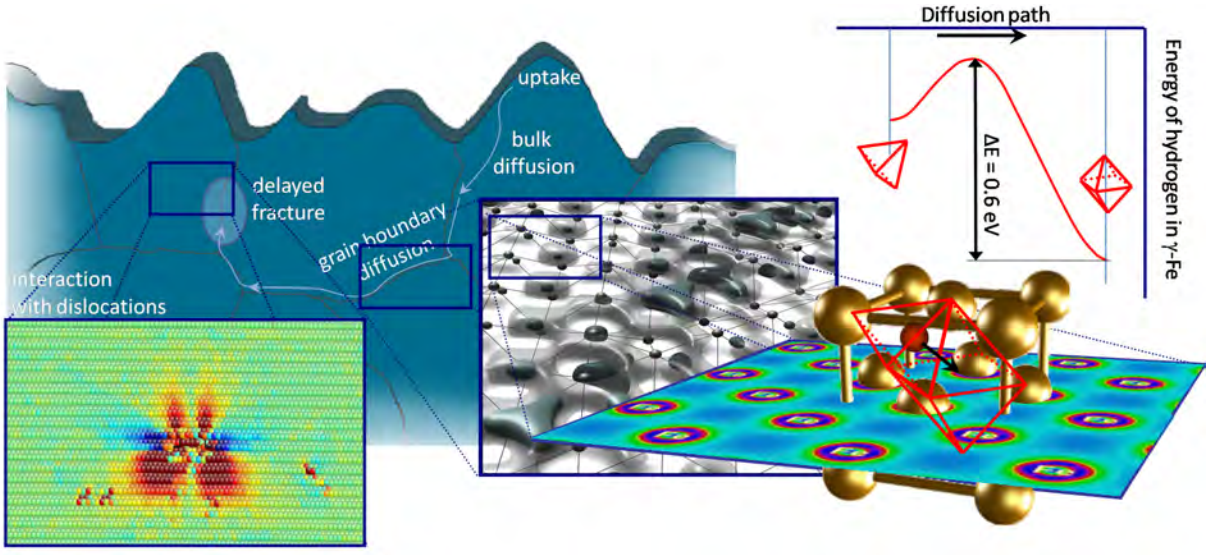


Fig. 8.1: The ASG Modelling addresses a variety of processes related to hydrogen embrittlement. This includes ab initio studies on the solution/diffusion of hydrogen in bulk phases/grain boundaries, kinetic Monte-Carlo simulations based on ab initio diffusion barriers and the investigation of atomistic mechanisms such as hydrogen enhanced local plasticity.

The Advanced Study Group (ASG) Modelling serves as a centre of competence for different concepts in materials modelling in order to support the research at ICAMS. At the same time the ASG contributes to the research of ICAMS with individual projects, which aim at a better understanding of steel properties on the atomistic scale by means of ab initio methods.

The ASG Modelling is situated at the Max-Planck-Institut für Eisenforschung in the department of Computational Materials Design (CM) of Prof. J. Neugebauer. Here, highly accurate simulation tools for the prediction of materials properties and processing, which are feasible on present day computers, are developed and applied. Within the department, the inherent multiscale character of realistic materials is considered in a bottom-up approach, motivated by the fact that the electronic scale is the fundamental scale which eventually controls processes on the macroscale. This approach has the advantage that it can be based on the well-established laws of quantum mechanics. It is therefore free of any adjustable or empirical parameters (ab initio), the elementary

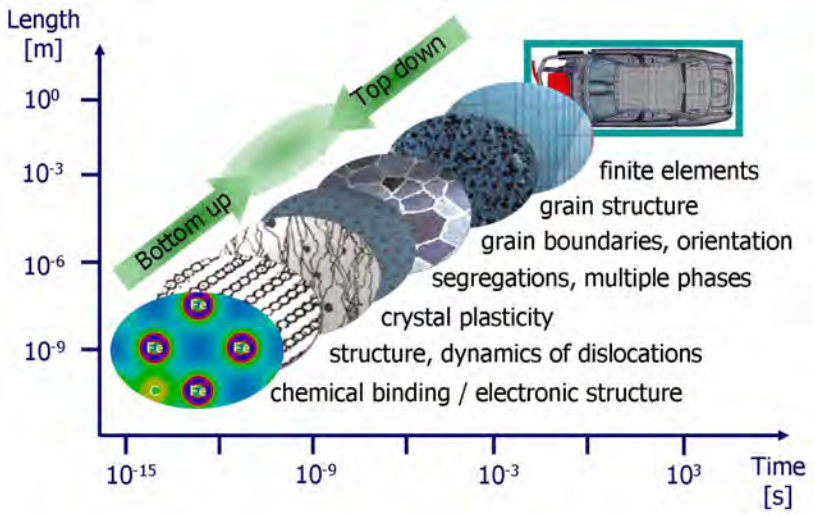


Fig. 8.2: Multiscale character of materials design. The ASG modelling follows a bottom-up approach, using well-established laws of quantum mechanics for the fundamental scale of individual electrons and atoms.

building blocks such as electrons and nuclei used in the simulations are identical to those in nature, and all equations defining the dynamics of these building blocks are well known.

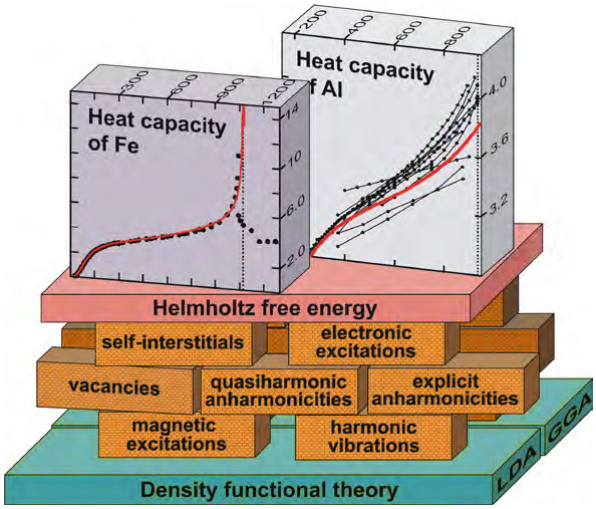


Fig. 8.3: Comparison of experimental (dots) and ab initio derived (red lines) heat capacities (in kB) of Fe and Al as a function of temperature (in K). The results are based on highly accurate methods developed in the CM department of MPIE to determine all relevant contributions to the Helmholtz free energy.

Advanced Study Group Input Data and Validation

9. Advanced Study Group Input Data and Validation

Prof. Dr.-Ing. Gunther Eggeler
Dr.-Ing. Jan Frenzel

The Advanced Study Group Input Data and Validation has a broad range of research objectives which benefit from interactions with other ICAMS groups. Most importantly, one focus lies on the processing, microstructures and mechanical behaviour of single crystal Ni-base superalloys at high temperatures. Our research activities on superalloys are conducted within the scope of the Collaborative Research Center SFB/Transregio 103 *Superalloy Single Crystals*. Superalloys represent key materials for modern gas turbines operating in electric power plants and aero engines because they withstand high mechanical loads at high temperatures (e.g. 1000 °C) and allow for high efficiencies and thus reduce emission of greenhouse gases.

Project B7 of the SFB/Transregio 103 investigates the formation of crystal defects, such as low angle grain boundaries and dislocations, which evolve during dendritic solidification of superalloy melts. We investigate how important solidification parameters affect the formation of these defects. For this type of research, it is important to evaluate the temperature fields close to the solid/liquid interface of the superalloy melt, since they govern

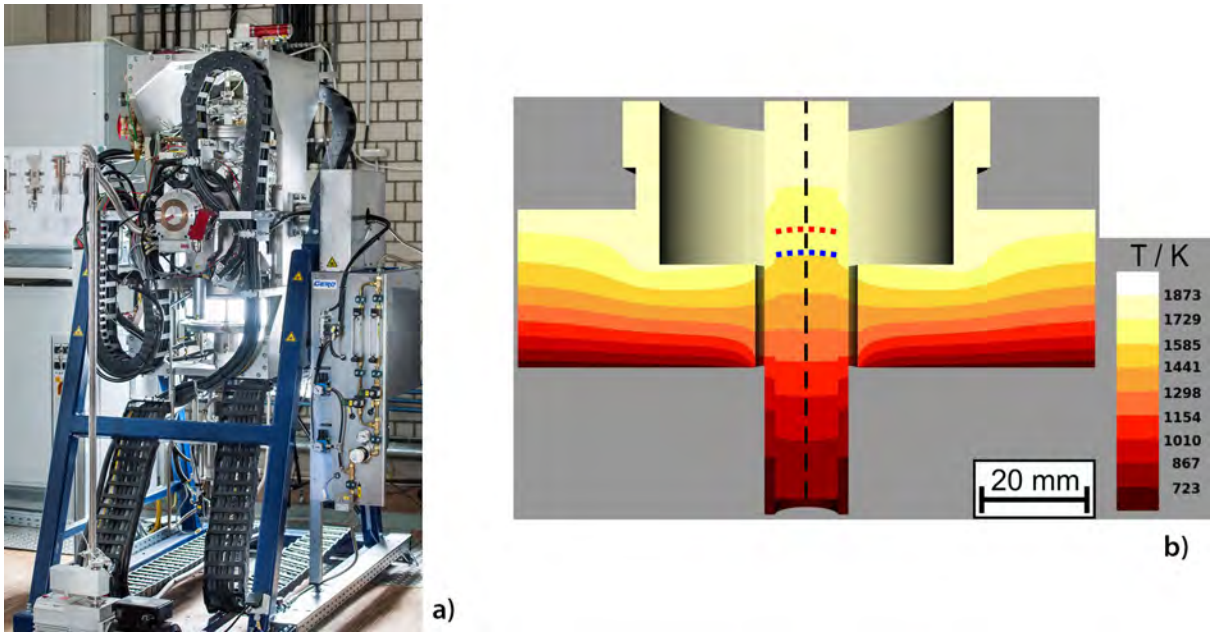


Fig. 9.1: Bridgman melting. a) Bridgman furnace (RUB), b) temperature distribution in the baffle region of the furnace. The dashed lines indicate liquidus (red) and solidus (blue) temperatures of the melt.

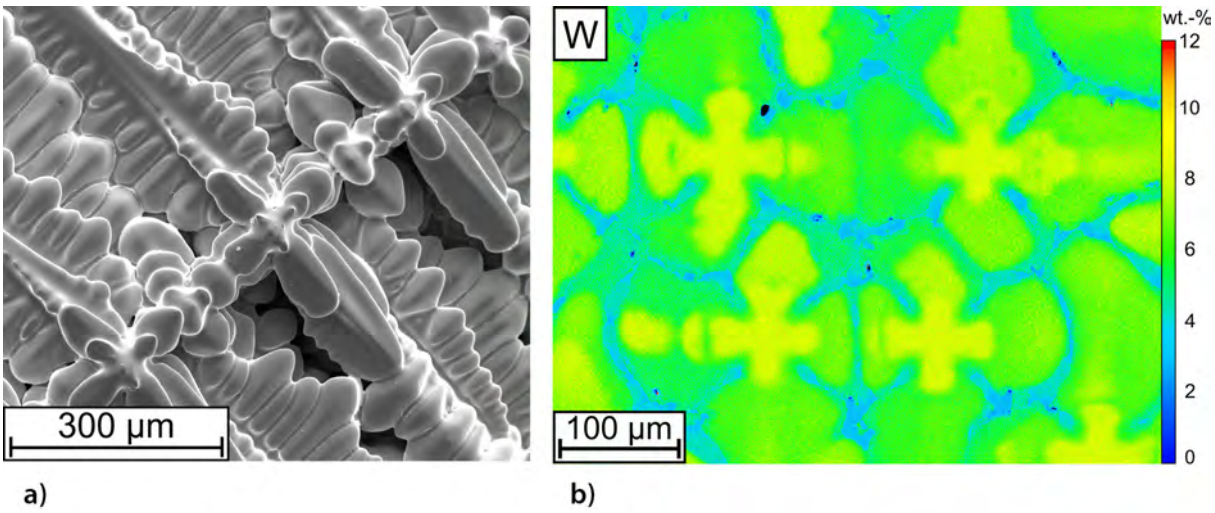


Fig. 9.2: Superalloy dendrites. a) Scanning electron microscopy image of free-standing dendrites, b) chemical information (Tungsten distribution) obtained by electron microprobe analysis.

solidification processes. An attempt was made to assess thermal fields by using numerical simulations. Helge Schaar and Ingo Steinbach (STKS) have developed a complex finite element model of the Bridgman furnace that allows evaluating temperature distributions on the basis of heat transport simulations. These simulations help to correlate the evolution of microstructures, as observed within solidification experiments, with solidification conditions that are only accessible by theoretical considerations. *Fig. 9.1* shows details on superalloy Bridgman melting. *Fig. 9.1a* shows a photograph of the melter, and *Fig. 9.1b* presents a colour-coded image of the temperature distribution in the lower part of the furnace. In this region, the superalloy melt contained in a cylindrical crucible (central vertical item in *Fig. 9.1b*) solidifies when being released from the heated zone of the furnace. A special focus lies on the microstructural characterization of the resulting samples by combining various techniques. *Fig. 9.2* exemplarily shows dendritic superalloy microstructures which resulted from directional solidification in our Bridgman furnace. *Fig. 9.2a* shows a scanning electron microscopy image of free-standing dendrites. *Fig. 9.2b* shows chemical information as obtained by electron microprobe analysis. The colour-coded map in *Fig. 9.2b* shows that dendrite cores contain higher Tungsten concentrations than interdendritic regions.

Fig. 9.3: A. Paulsen (on the very right) demonstrating a high temperature shape memory spring actuator (mounted in a small test frame) to Prof. P. Sittner, Dr. G. Firstov, Prof. H. J. Maier and Dr. E. Pagounis at the HTSMA *conference in Wildbad-Kreuth.*

Members of the ASG also investigate high-temperature shape memory alloys within the framework of the DFG research unit FOR 1766. After a successful evaluation in 2015, the DFG research unit FOR 1766 is now in its second funding period. Shape memory effects rely on a reversible martensitic transformation, where a high-temperature phase (austenite) transforms into a low-temperature phase (martensite) on cooling. The reverse transformation occurs upon heating. Shape memory alloys exhibit fascinating properties: They are able to re-establish their initial geometry after a deformation which significantly exceeds conventional elastic strains. Recently, good progress was made on Titanium-Tantalum-based SMAs. *Fig. 9.3* shows Alexander Paulsen presenting a Ti-Ta-based demonstrator setup at the *HTSMA* conference in Wildbad-Kreuth.

Advanced Study Group Processing and Characterization

10. Advanced Study Group Processing and Characterization

Prof. Dr.-Ing. Wolfgang Bleck
Prof. Dr.-Ing. Sebastian Münstermann
Dr. Ulrich Prahl

The research activities of the ASG Processing and Characterization located at the Institut für Eisenhüttenkunde (IEHK) involve the major topics materials characterization, advanced computer simulation of materials, materials processing, and fracture mechanics. The ultimate aim is to understand the mechanisms behind the physical, mechanical, and microstructural properties of steels, to be able to improve their macroscopic behaviour through transformations and variations of the microscopic phases, and to design advanced solutions for steel production, processing and application. The scientific approach of the institute is to use a combination of different mechanical and physical testing methods with advanced numerical approaches in order to investigate the bulk properties of different iron-based alloys at sub-zero temperatures as well as room and elevated temperatures.

Using a suitable combination of microstructural design, process optimization, and mechanical testing, it becomes possible to introduce more efficient process parameters, innovative applications and new materials. The simulation work focuses on the integrative numerical modelling of the evolution of microstructures during processing on different scales.

The objectives are to combine physical and phenomenological approaches, to evaluate modelling approaches, to describe processes and process chains by numerical means, and to predict the evolution of microstructures and properties by using combined thermodynamical and FEM calculations of representative volume elements (RVEs) on the microstructural scale. By means of simulation, it is aimed to develop materials and processes, to design and to optimise production parameters and to predict materials behaviour in relation to the microstructural description.

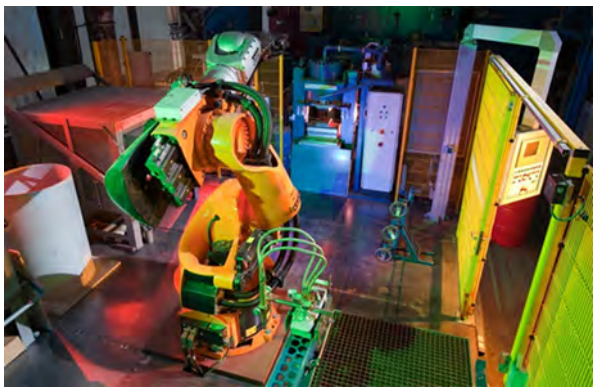


Fig. 10.1: SemiProductSimulationCenter at IEHK.

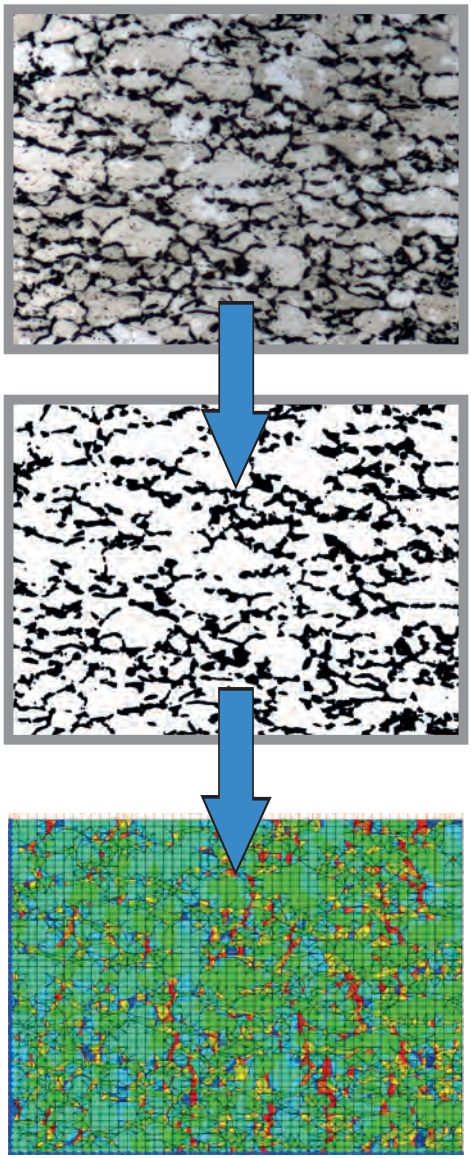


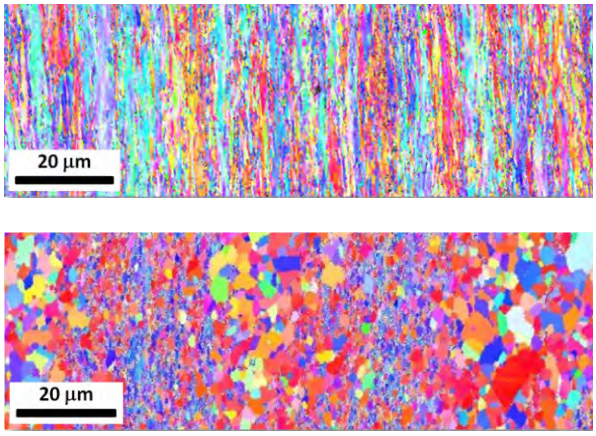
Fig. 10.2: Modelling of crack evolution.

Advanced Study Group Diffusion and Microstructure Analysis

11. Advanced Study Group Diffusion and Microstructure Analysis

Prof. Dr.-Ing. Gerhard Wilde
Dr. Sergiy Divinski
Dr. Harald Rösner

The Advanced Study Group Diffusion and Microstructure Analysis (DMA) is located at the Chair for Materials Physics of the Institute of Materials Physics at Westfälische Wilhelms-Universität Münster. The ASG employs a range of complementing experimental methods to analyse the underlying physical mechanisms and microstructural origins of macroscopic materials behaviour. Specific emphasis is on the coupled analysis of grain boundary diffusion, detailed characterisation of the atomic structure of these internal interfaces, and microstructure evolution in deformed materials. Furthermore, we focus on the analysis of defects and defect interactions by combining electron microscopy on different length scales with calorimetry and atomic mobility analyses. Moreover, nucleation and growth phenomena as well as phase transformations are also in the centre of our interest. The experimental analyses generate input data for the modelling work on different length scales, which is carried out at ICAMS. The data are provided for in-depth comparison with and critical verification of the results obtained by computational analyses.



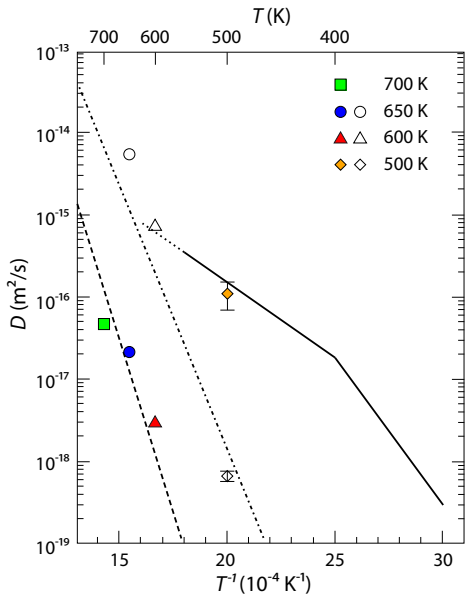


Fig. 11.1: Microstructure of ECAP-processed Ni in the as-prepared state (top), and after annealing at 700 K for 17 hours (middle); the Arrhenius plot for the measured self-diffusion coefficients D of ^{63}Ni in ECAP-Ni (bottom). The Ni diffusion rates in ECAP-processed 99.6 wt% pure Ni (symbols and solid lines) are shown against Ni grain boundary diffusion coefficients in coarse-grained Ni of 99.6 wt% (dashed line) and 99.999 wt% (dashed-dotted line) purities.

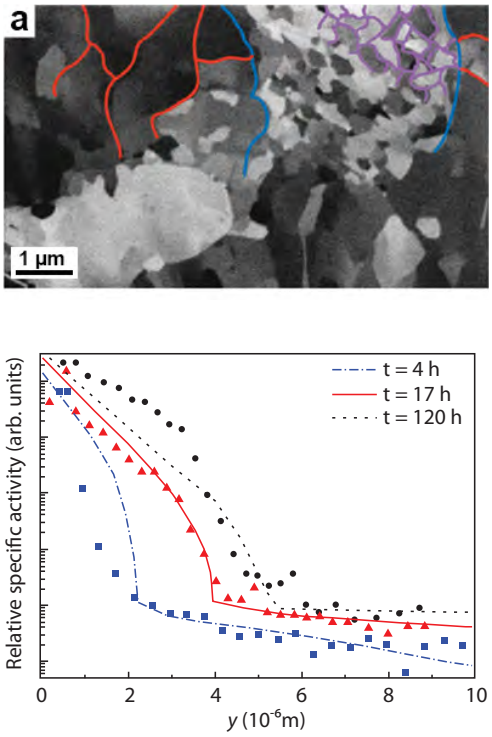


Fig. 11.2: Microstructure and grain boundary types in ECAP-processed Ni in the course of heterogeneous recrystallisation (top) and the penetration profiles of ^{63}Ni as a function of the diffusion time t (bottom).

Examples for collaboratively addressed topics are:

- Defect dynamics at precipitates in severely deformed Al-based alloys
- Grain boundary diffusion in ferromagnetic steels
- Oxidation and nitridation kinetics of ODS steel
- Recrystallisation and grain growth in severely deformed Ni
- Thermodynamics and diffusion in high-entropy alloys
- Shear bands in metallic glasses

The Advanced Study Group Diffusion and Microstructure Analysis is actively involved in the DFG-funded priority program *Strong coupling of thermo-chemical and thermo-mechanical states in applied materials* (SPP1713), which is coordinated by ICAMS and started in 2014.

Research Highlights

12. Research Highlights

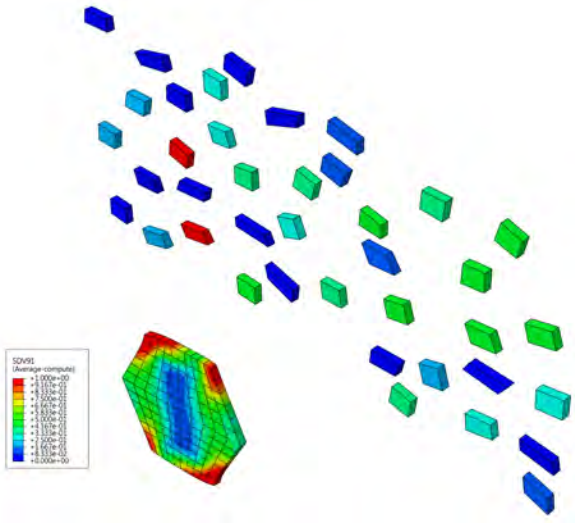
2015

A study of deformation and phase transformation coupling for TRIP-assisted steels

A. Ma, A. Hartmaier

International Journal of Plasticity, **64**, 40-55 (2015)

A constitutive model for Transformation Induced Plasticity (TRIP) assisted steels is proposed that considers the elastic–plastic deformation of ferrite and austenite, the austenite–martensite phase transformation and the elastic deformation of martensite. Within this model, an explicit relation between martensite nucleation and plastic deformation within an austenite grain has been established based on the inverse Nishiyama–Wassermann (NW) relationship. In particular, strain-induced martensite nucleation and stress-assisted martensite growth have been included in one model with the help of a thermodynamic principle. With this model, we found consistently with experiment that the TRIP effect enhances the effective work hardening rate and hence is beneficial for improving strength and ductility of steels. The mechanical anisotropy produced by stress-assisted and strain-induced phase transformations are significantly different. Furthermore, we observed that austenite grains transform to martensite more quickly under tension than under compression.



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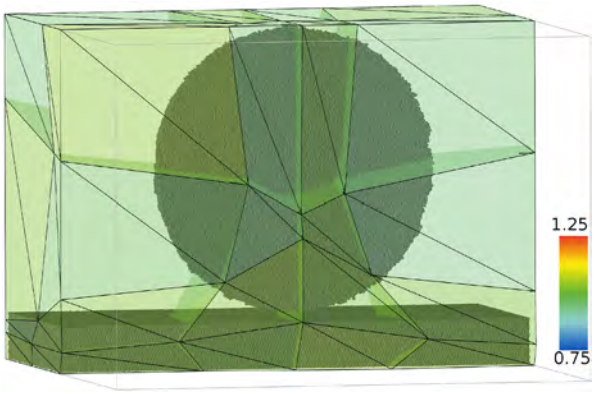
Adaptive dynamic load-balancing with irregular domain decomposition for particle simulations

C. Begau, G. Sutmann

Computer Physics Communications, **190**, 51-61 (2015)

We present a flexible and fully adaptive dynamic load-balancing scheme, which is designed for particle simulations of three-dimensional systems with short ranged interactions. The method is based on domain decomposition with non-orthogonal non-convex domains, which are constructed based on a local repartitioning of computational work between neighbouring processors. Domains are dynamically adjusted in a flexible way under the condition that the original topology is not changed, i.e. neighbour relations between domains are retained, which guarantees a fixed communication pattern for each domain during a simulation. Extensions of this scheme are discussed and illustrated with examples, which generalise the communication patterns and do not fully restrict data exchange to direct neighbours. The proposed method relies on a linked cell algorithm, which makes it compatible with existing implementations in particle codes and does not modify the underlying algorithm for calculating the forces between particles.The method has been implemented into the molecular dynamics community code IMD and performance has been measured for various molecular dynamics simulations of systems representing realistic problems from materials science. It is found that the method proves to balance the work between processors in simulations with strongly inhomogeneous and dynamically changing particle distributions, which results in a significant increase of the efficiency of the parallel code compared both to unbalanced simulations and conventional load-balancing strategies.



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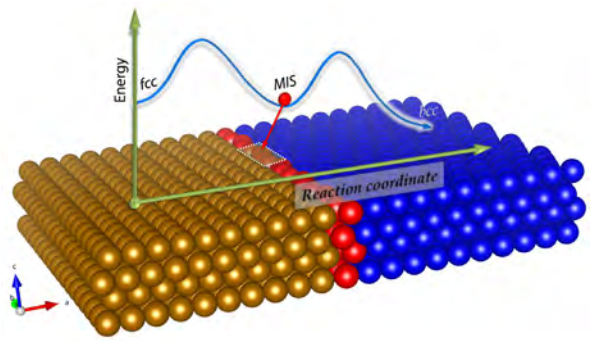
Structural transformations among austenite, ferrite and cementite in Fe-C alloys: A unified theory based on ab initio simulations

X. Zhang, T. Hickel, J. Rogal, S. Fähler, R. Drautz, J. Neugebauer

Acta Materialia, **99**, 281-289 (2015)

Structural transformations in Fe–C alloys are decisive for the mechanical properties of steels, but their modelling remains a challenge due to the simultaneous changes in Fe lattice and redistribution of C. With a combination of the orientation relationships between austenite, ferrite and cementite, we identify a metastable intermediate structure (MIS), which can serve as a link between the three phases. Based on this framework, different mechanisms depending on the local conditions (C concentration, strain, magnetism) are revealed from ab initio nudged elastic band simulations, which allow us to construct a unified theory for the structural transformations among austenite, ferrite and cementite.

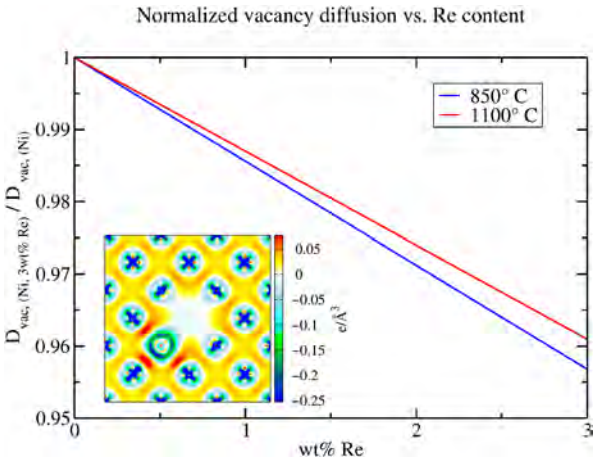


Schematic representation of the metastable intermediate structure (MIS, red) that serves as an interface reconstruction simultaneously providing a lattice correspondence between austenite (fcc, gold), ferrite (bcc, blue) and cementite in Fe-C alloys.

On the role of Re in the stress and temperature dependence of creep of Ni-base single crystal superalloys

P. Wollgramm, H. Buck, K. Neuking, A. B. Parsa, S. Schuwalow, J. Rogal, R. Drautz, G. Eggeler

Materials Science and Engineering A, **628**, 382-395 (2015)



Normalized vacancy diffusion coefficient in Ni as a function of Re solute concentration for two different temperatures. The inset shows the valence charge density of a Re solute atom next to a vacancy in Ni.

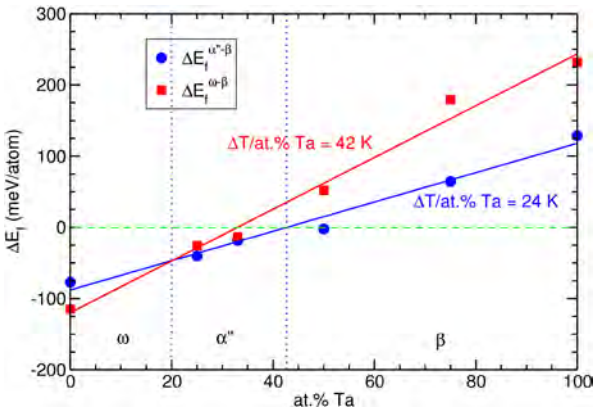
In the present study, we investigate the creep behaviour of a Ni-base single crystal superalloy. We evaluate the stress and temperature dependence of the minimum creep rate, which shows a power law type of stress dependence (characterized by a stress exponent n) and an exponential type of temperature dependence (characterized by an apparent activation energy Q_{app}). Under conditions of high temperature (1323 K) and low stress (160 MPa) creep, n and Q_{app} are determined as 5.3 and 529 kJ/mol, respectively. For lower temperatures (1123 K) and higher stresses (600 MPa), the stress exponent n is higher (8.5) while the apparent activation energy of creep is lower (382 KJ/mol). We show that there is a general trend: stress exponents n increase with increasing stress and decreasing temperature, while higher apparent activation energies are observed for lower stresses and higher temperatures. We use density functional theory (DFT) to calculate the activation energy of diffusion for Re in a binary Ni-Re alloy with low Re-concentrations. The resulting energy is almost a factor 2 smaller than the apparent activation energy of creep. We explain why it is not straightforward to rationalize the temperature dependence of creep merely on the basis of the diffusion of one alloying element. We show that the evolution of the microstructure must be considered as well.

Martensitic transformation between competing phases in Ti–Ta alloys: A solid-state nudged elastic band study

T. Chakraborty, J. Rogal, R. Drautz

Journal of Physics: Condensed Matter, **27**, 115401 (2015)

A combined density functional theory and solid-state nudged elastic band study is presented to investigate the martensitic transformation between β → (α″, ω) phases in the Ti–Ta system. The minimum energy paths along the transformation are calculated and the transformation mechanisms as well as relative stabilities of the different phases are discussed for various compositions. The analysis of the transformation paths is complemented by calculations of phonon spectra to determine the dynamical stability of the β, α″, and ω phase. Our theoretical results confirm the experimental findings that with increasing Ta concentration there is a competition between the destabilisation of the α″ and ω phase and the stabilisation of the high-temperature β phase.

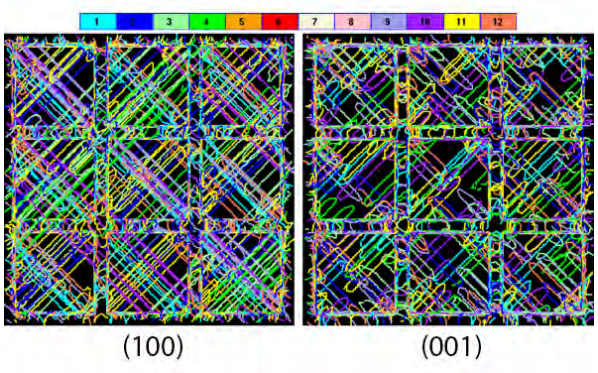


Difference in formation energies between the martensite α and austenite β phase (blue circles) as well as between the ω and austenite phase (red squares) in Ti-Ta high-temperature shape memory alloys as a function of Ta concentration. Vertical lines mark the stability region of each phase.

Influence of misfit stresses on dislocation glide in single crystal superalloys: A three-dimensional discrete dislocation dynamics study

S. Gao, M. Fivel, A. Ma, A. Hartmaier

Journal of the Mechanics and Physics of Solids, **76**, 276-290 (2015)



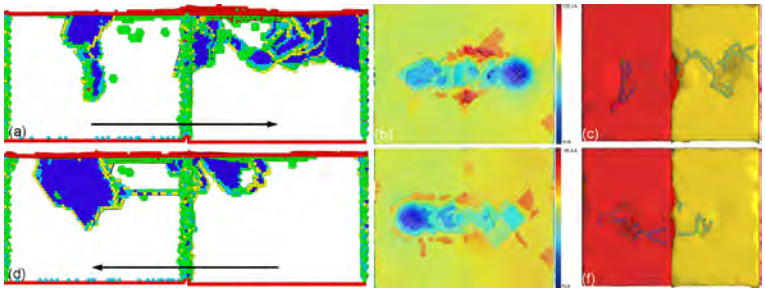
Dislocation configurations in matrix channels obtained for a simulation with a negative lattice mismatch ratio of δ=−0.005. Dislocations are viewed in projections on (100) and (001) crystallographic planes, as given in the figures, after simulation times of 15 ns.

In the characteristic γ/γ' microstructure of single crystal superalloys, misfit stresses occur due to a significant lattice mismatch of those two phases. The magnitude of this lattice mismatch depends on the chemical composition of both phases as well as on temperature. Furthermore, the lattice mismatch of γ and γ' phases can be either positive or negative in sign. The internal stresses caused by such lattice mismatch play a decisive role for the micromechanical processes that lead to the observed macroscopic athermal deformation behaviour of these high-temperature alloys. Three-dimensional discrete dislocation dynamics (DDD) simulations are applied to investigate dislocation glide in γ matrix channels and shearing of γ' precipitates by superdislocations under externally applied uniaxial stresses, by fully taking into account internal misfit stresses. Misfit stress fields are calculated by the fast Fourier transformation (FFT) method and hybridized with DDD simulations. For external loading along the crystallographic [001] direction of the single crystal, it was found that the different internal stress states for negative and positive lattice mismatch result in non-uniform dislocation movement and different dislocation patterns in horizontal and vertical γ matrix channels. Furthermore, positive lattice mismatch produces a lower deformation rate than negative lattice mismatch under the same tensile loading, but for an increasing magnitude of lattice mismatch, the deformation resistance always diminishes. Hence, the best deformation performance is expected to result from alloys with either small positive, or even better, vanishing lattice mismatch between γ and γ' phase.

Atomistic investigation of wear mechanisms of a copper bi-crystal

J. Zhang, C. Begau, L. Geng, A. Hartmaier

Wear, **332-333**, 941-948 (2015)



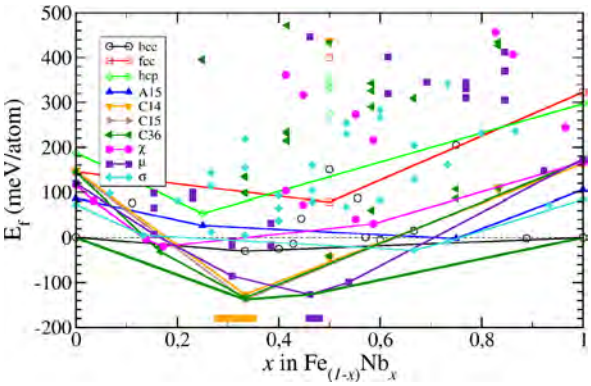
Defect structures, surface morphologies, and grain profiles.

In the present work, we investigate the wear mechanisms of a Cu bi-crystal containing a random high angle grain boundary by means of molecular dynamics simulations. The underlying deformation behaviour of the material is analyzed and further related to the observed characteristics of mechanical response and resulting morphology of the worn surface. In particular, the grain boundary-associated mechanisms are characterized by advanced analysis techniques for lattice defects. Our simulation results indicate that in addition to dislocation slip and dislocation-grain boundary interactions, grain boundary migration plays an important role in the plastic deformation of the Cu bi-crystal. It is found that the wear behaviour of Cu depends on the crystallographic orientation of the worn surface and can be altered quite significantly by the presence of a grain boundary.

Structural stability of Fe-based topologically close-packed phases

A. C. Ladines, T. Hammerschmidt, R. Drautz

Intermetallics, **59**, 59-67 (2015)



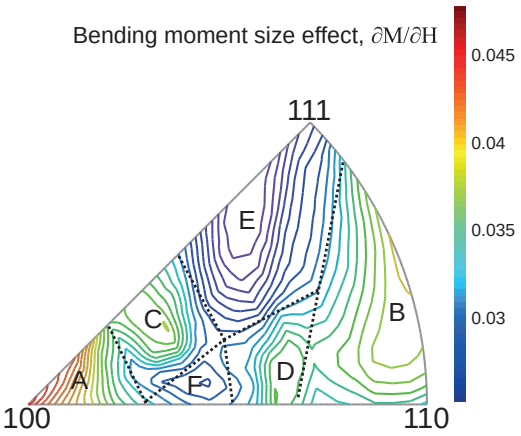
Formation energy of topologically close-packed phases and bcc/fcc/hcp solid solutions in the Fe-Nb system. The overall convex hull indicates the stability of the Fe_2Nb Laves phases and the Fe_7Nb_6 mu-phase that are also observed experimentally.

Precipitates of topologically close-packed (TCP) phases play an important role in hardening mechanisms of high-performance steels. We analyze the influence of atomic size, electron count, magnetism and external stress on TCP phase stability in Fe-based binary transition metal alloys. Our density-functional theory calculations of structural stability are complemented by an analysis with an empirical structure map for TCP phases. The structural stability and lattice parameters of the Fe–Nb/Mo/V compounds are in good agreement with experiment. The average magnetic moments follow the Slater-Pauling relation to the average number of valence-electrons and can be rationalized in terms of the electronic density of states. The stabilizing effect of the magnetic energy, estimated by additional non-magnetic calculations, increases as the magnetic moment increases with band filling for the binary systems of Fe and early transition metals. For the case of Fe_2Nb, we demonstrate that the influence of magnetism and external stress is sufficiently large to alter the energetic ordering of the closely competing Laves phases C14, C15 and C36. We find that the A15 phase is not stabilized by atomic-size differences, while the stability of C14 is increasing with increasing difference in atomic size.

Investigating the influence of crystal orientation on bending size effect of single crystal beams

S. Gupta, A. Ma, A. Hartmaier

Computational Materials Science, **101**, 201–210 (2015)



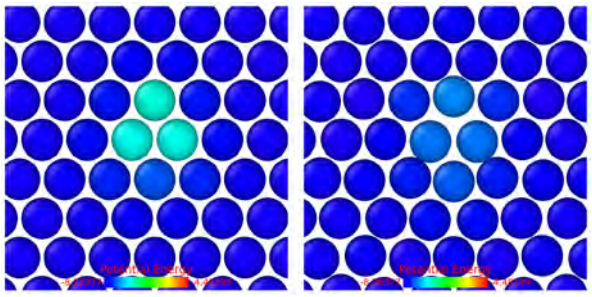
Graphic reprinted from Computational Materials Science, 101, Satyapriya Gupta, Anxin Ma, Alexander Hartmaier, Investigation of the influence of crystal orientation on bending size effect of single crystal beams, 201-210, © 2015, with permission from Elsevier.

Influence of crystal orientation on bending size effect has been numerically investigated for single crystal beams. This work is inspired by the experimental observations of Hayashi et al. (2011), where they observed a significant difference in bending size effect for two different crystal orientations. We have used a higher order non-local crystal plasticity model which can account for different hardening contributions by SSDs (statistically stored dislocations) and GNDs (geometrically necessary dislocations) simultaneously. It was found that strain hardening together with an additional kinematic hardening caused by accumulation of GNDs and the number of activated slip systems can be seen as the origin of the orientation dependence of bending size effect. We have also observed a pronounced orientation dependence of spring back size effect, which can be explained on the basis of number of the activated slip systems and equivalent plastic strain. Simulation results showing enhanced or diminished bending size effect for different crystal orientations reveal the importance of crystal orientation for precise micro-bending operations.

Parallel bond order potentials for materials science simulations

C. Teijeiro Barjas, T. Hammerschmidt, R. Drautz, G. Sutmann

Proceedings of the 4th International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering (2015)



Change of potential energy during relaxation of a 1/2[111] screw dislocation in bcc-W computed by parallel computations with analytic bond-order potentials. The colour coding indicates atom-resolved binding energy.

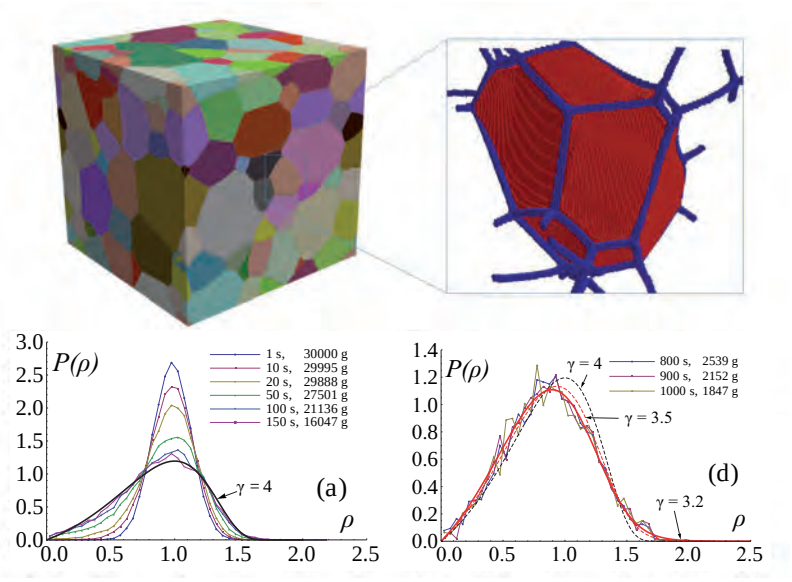
The computation of interatomic interactions in materials science is a challenging problem, because of the need for an accurate description of different bonding situations. Density functional theory (DFT) and tight binding (TB) provide good approximations to the problem but have high computational complexity, which limits the size of the systems to be studied. Analytic bond-order potentials (BOPs) provide a coarse-grained computation of interatomic interactions derived from DFT and TB in order to obtain satisfactory approximations, with an order-N increase in the simulation time as the system size grows. Even though BOPs are significantly less expensive than first principle methods, analytic BOPs require an efficient implementation in order to obtain good scalability for large systems. This paper presents a performance evaluation of a parallel implementation of a BOP code, with a description of the most time consuming tasks, and basic concepts for a parallelisation of the simulation. The main contributions of this paper are (1) the analysis of an optimized simulation code in terms of its different routines, (2) the implementation of parallel algorithms that take advantage of the nature of the simulation to obtain high scalability, (3) a performance evaluation of the parallel code on average-sized systems and the proposal of best practices for future developments, and (4) the example of integration of the routine for the precise computation of energies and forces in a molecular dynamics (MD) code.

Geometrical grounds of mean field solutions for normal grain growth

R. Darvishi Kamachali, A. Abbondandolo, K.F. Siburg, I. Steinbach

Acta Materialia, **90**, 252–258 (2015)

The classic mean field approach for normal grain growth in polycrystalline materials is revisited. We re-drive and study possible self-similar solutions and show that the grain size distribution can be determined only by the geometry of neighbouring grains for any given configuration. In three dimensions, it is shown that a single index $\langle r\rangle^2/\langle r^2\rangle$ can represent the geometrical characteristic of grains and has a one-to-one relationship with the mean field parameter γ. We reinvestigate the results of our recent phase-field study in the light of new analytical results and find a value γ≈3.5–3.2 for the stable regime.

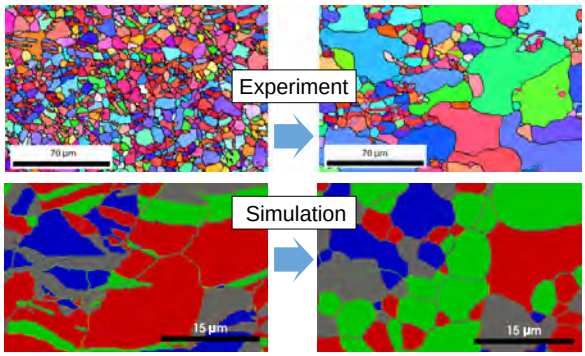


The mean field theory of grain growth has been revisited: We have shown the possibility of multiple self similar solutions for normal grain growth that only depend on the geometry of neighbouring grains. The figure compares simulation results with analytical solutions.

Texture evolution in deformed AZ31 magnesium sheets: Experiments and phase-field study

R. Darvishi Kamachali, S. Kim, I. Steinbach

Computational Materials Science, **104**, 193-199 (2015)



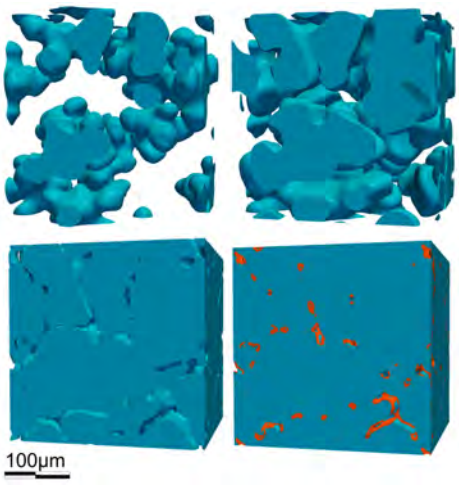
The mechanism of texture evolution in AZ31 thin sheets has been revealed during sequential deformation and annealing processing. Using phase-field simulations, the role of stored mechanical energies due to dislocations on the recrystallization has been clarified. The figure shows a comparison between simulation and experiment before and after annealing.

Experimental and phase-field studies are performed to investigate mechanisms of preferential growth which lead to improved formability in AZ31 Mg sheets. A compression/annealing treatment is specialized to modify the initial texture in thin sheets. The texture and stress states of materials are studied via electron back scattered diffraction (EBSD) technique before and after annealing. Using the EBSD data on microstructure and residual stresses, a phase-field model is constructed to simulate the texture evolution after initial compression. The results suggest that the residual-stresses induced by in-plane compression are the main driving force for recrystallization and grain growth. The inhomogeneous stress distribution leads to preferential growth of $\{21\bar{1}0\}$ texture along the normal to the sheet, which are at lowest stress state, at the expense of initial basal texture. Limited mobility of twin boundaries changes the mixture of textures but the non-basal textures are still preferred. The formability tests confirm a significant enhancement of the final product compared to as-received sheets.

Dual-scale phase-field simulation of Mg-Al alloy solidification

A. Monas, O. Shchyglo, D. Höche, M. Tegeler, I. Steinbach

IOP Conference Series: Materials Science and Engineering, **84,** 012069 (2015)



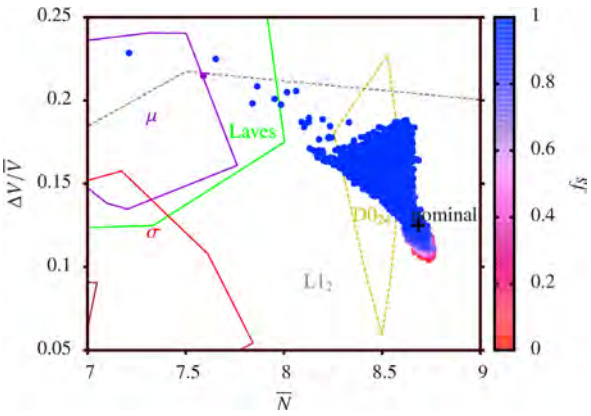
Results of the large-scale 3D simulation of nucleation and growth of primary α-phase (blue) followed by the nucleation and growth of secondary interdendritic eutectic β-phase (orange).

Phase-field simulations of the nucleation and growth of primary α-Mg phase as well as secondary β-phase of a Mg-Al alloy are presented. The nucleation model for α- and β-Mg phases is based on the "free growth model" by Greer et al. After the α-Mg phase solidification we study a divorced eutectic growth of α- and β-Mg phases in a zoomed-in melt channel between α-phase dendrites. The simulated cooling curves and final microstructures of α-grains are compared with experiments. In order to further enhance the resolution of the interdendritic region, a high-performance computing approach has been used allowing significant simulation speed gain when using supercomputing facilities.

Microsegregation and precipitates of an as-cast Co-based superalloy - microstructural characterization and phase stability modelling

J. Koßmann, C.H. Zenk, I. Lopez-Galilea, S. Neumeier, A. Kostka, S. Huth, W. Theisen, M. Göken, R. Drautz, T. Hammerschmidt

Journal of Materials Science, **50**, 6329-6338 (2015)



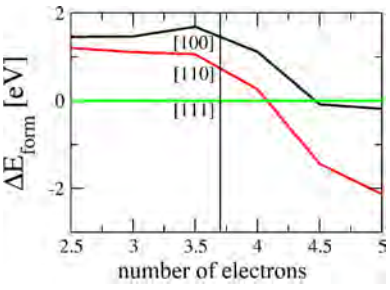
Analysis of experimentally observed variation of chemical composition during solidification of Co-base superalloy ERBO-Co0 in terms of a structure map using average number of valence electrons (N) and differences in atomic size (V). With increasing fraction of solidification (fs), the local chemical compositions reach the stability regions of topologically close-packed phases.

The demand for increased efficiency of industrial gas turbines and aero engines drives the search for the next generation of materials. Promising candidates for such new materials are Co-based superalloys. We characterize the microsegregation and solidification of a multi-component Co-based superalloy and compare it to a ternary Co–Al–W compound and to two exemplary Ni-based superalloys by combining the experimental characterization of the as-cast microstructures with complementary modelling of phase stability. On the experimental side, we characterize the microstructure and precipitates by electron microscopy and energy-dispersive X-ray spectroscopy and determine the element distributions and microsegregation coefficients by electron probe microanalysis (EPMA). On the modelling side, we carry out solidification simulations and a structure map analysis in order to relate the local chemical composition with phase stability. We find that the microsegregation coefficients for the individual elements are very similar in the investigated Co-based and Ni-based superalloys. By interpreting the local chemical composition from EPMA with the structure map, we effectively unite the set of element distribution maps to compound maps with very good contrast of the dendritic microstructure. The resulting compound maps of the microstructure in terms of average band filling and atomic-size difference explain the formation of topologically close-packed phases in the interdendritic regions. We identify B2, C14, and D024 precipitates with chemical compositions that are in line with the structure map.

Bond-order potentials: Derivation and parameterization for refractory elements

R. Drautz, T. Hammerschmidt, M. Čák, D. G. Pettifor

Modelling and Simulation in Materials Science and Engineering, **23**, 74004 (2015)



Influence of the d-electron count on the energetic ordering of the [111],[110] and [100] self-interstitial defects in Nb as obtained with an analytic bond-order potential.

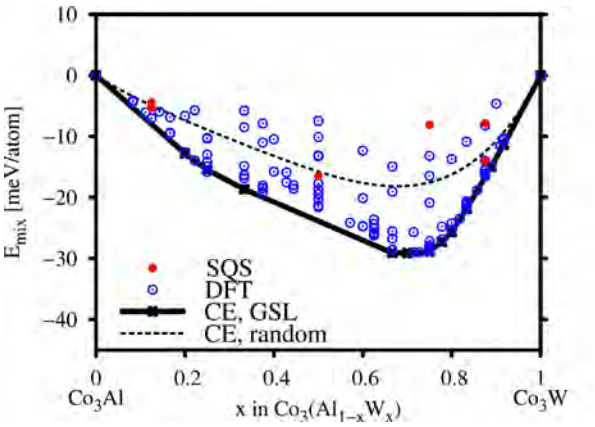
The bond-order potentials are derived from density functional theory by a systematic coarse graining of the electronic structure. Within their functional form the bond-order potentials comprise covalent bond formation, charge transfer and magnetism. We review the derivation of the bond-order potentials from density functional theory and discuss their application to the simulation of refractory transition metals. We show that the derived functional form of the bond-order potentials ensures the transferability of the potentials to atomic environments that have not been taken into account in the parameterization.

Solubility and ordering of Ti, Ta, Mo and W on the Al sublattice in $L1_2$-Co_3Al

J. Koßmann, T. Hammerschmidt, S. Maisel, S. Müller, R. Drautz

Intermetallics, **64**, 44-50 (2015)

Co–Al–W-based alloys are promising new materials for high-temperature applications. They owe their high-temperature strength to hardening by ternary $L1_2$-$Co_3(Al_{1-x}W_x)$ precipitates, which may form even though binary Co_3Al is not stable. In the current work, density functional theory calculations are performed to study the solubility and ordering of the transition metals W, Mo, Ti, and Ta at the Al sublattice in $L1_2$-Co_3Al. The sublattice disorder is modelled with a newly parametrized cluster expansion and compared to results using special quasi-random structures. Our results for W and Mo show that the mixing energy exhibits a minimum at approximately x = 0.7. However, the computed small values of the mixing energies indicate that W and Mo atoms are fully disordered with the Al atoms at low temperatures already. For Ti and Ta we find no sizeable driving force for ordering with the Al atoms. The computed solubilities on the Al sublattice obtained are in the range of 40–80 meV/atom for W and Mo and less than 25 meV/atom for Ti and Ta.

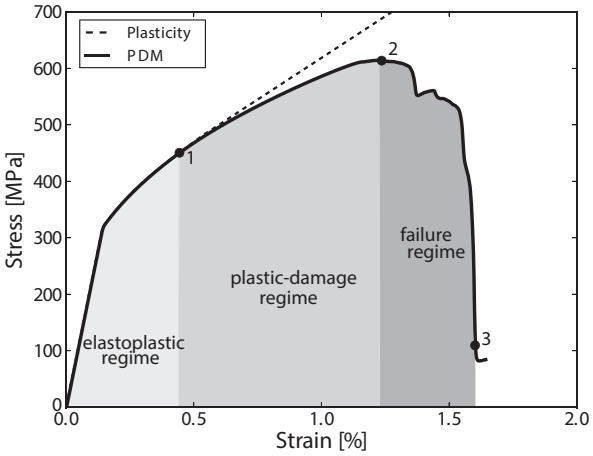


Energy of mixing (in eV/atom) of Al and W on the Al-sublattice of $Co_3(Al/W)$ as obtained from density-functional theory calculations. The disorder is treated by special quasi-random structures (SQS) and a cluster expansion (CE) showing the ground-state line (GSL) and the random alloy.

Formulation of nonlocal damage models based on spectral methods for application to complex microstructures

M. Boeff, P. S. Engels, A. Ma, A. Hartmaier

Engineering Fracture Mechanics, **147**, 373-387 (2015)



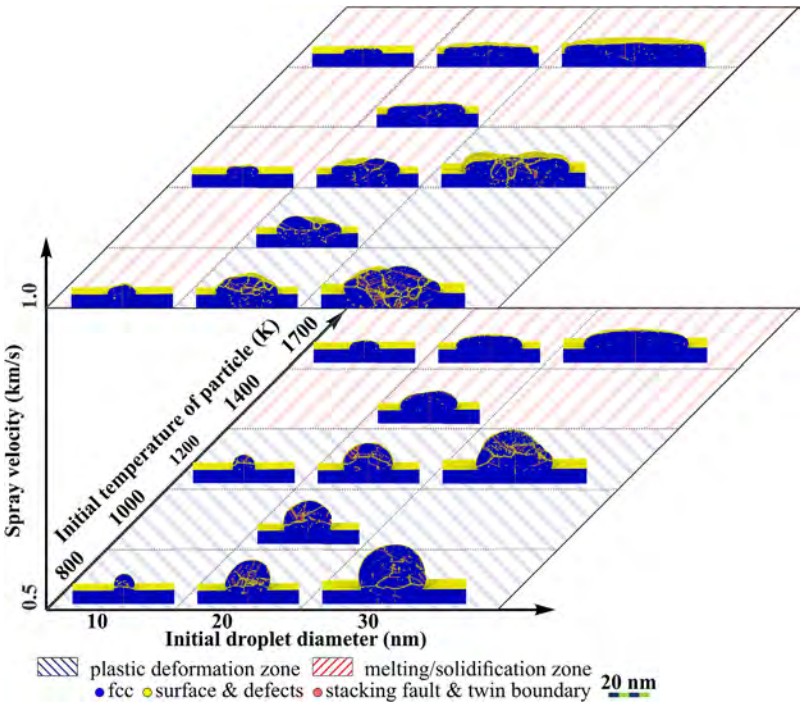
Graphic reprinted from Engineering Fracture Mechanics, 147, Martin Boeff, Florian Gutknecht, Philipp S. Engels, Anxin Ma, Alexander Hartmaier, Formulation of nonlocal damage models based on spectral methods for application to complex microstructures, 373-387, © 2015, with permission from Elsevier.

The increasing interest in modelling local deformations and damage evolution within materials with complex microstructures leads to an increasing demand for efficient numerical methods. A method designed to study damage evolution within the microstructure should be able to deal with complex geometries and to capture system sizes that are large enough to rectify the assumptions made when naming them representative volume elements (RVEs). We introduce a non-local damage model into the framework of a spectral solver and study initiation and evolution of damage on the microstructural scale, where regions susceptible to damage are identified.

Large scale molecular dynamics simulation of microstructure formation during thermal spraying of pure copper

T. Wang, C. Begau, G. Sutmann, A. Hartmaier

Surface and Coatings Technology, **280**, 72-80 (2015)



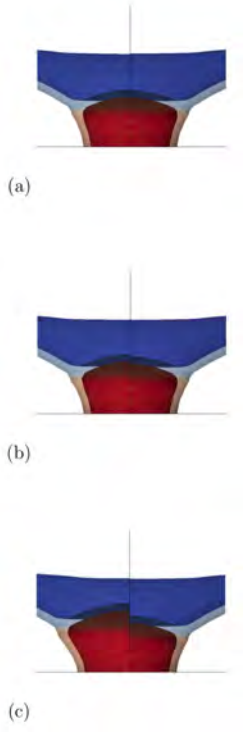
Microstructural diagram obtained from MD simulations with different spraying velocities, diameters and initial temperatures of the particles.

Thermal spray processes are widely used for the manufacture of advanced coating systems, e.g. metallic coatings for wear and corrosion protection. The desired coating properties are closely related to the microstructure, which is highly influenced by the processing parameters, such as temperature, size and velocity of the sprayed particles. In this paper, large-scale Molecular Dynamics simulations are conducted to investigate the microstructure formation mechanisms during the spraying process of hot nano-particles onto a substrate at room temperature, using pure copper as a benchmark material representative for a wider class of face-centered-cubic metals. To evaluate the influence of processing parameters on the coating morphology, a number of simulations are performed in which the initial temperature, size and velocity of copper particles are systematically varied in order to investigate the thermal and microstructural evolution during impaction. Two distinct types of microstructural formation mechanisms, resulting in different coating morphologies, are observed in the present investigation, which are either governed by plastic deformation or by the process of melting and subsequent solidification. Furthermore, a thermodynamically motivated model as a function of the particle temperature and velocity is developed, which predicts the microstructural mechanisms observed in the simulations. The results provide an elementary insight into the microstructure formation mechanisms on an atomistic scale and can serve as basic input for continuum modelling of thermal spray process.

Simulations of the eutectic transformations in the platinum–carbon system

A. Monas, P. Bloembergen, W. Dong, O. Shchyglo, I. Steinbach

International Journal of Thermophysics, **36**, 3366-3383 (2015)



Pt-C solidification simulation results with different amounts of Au impurity.

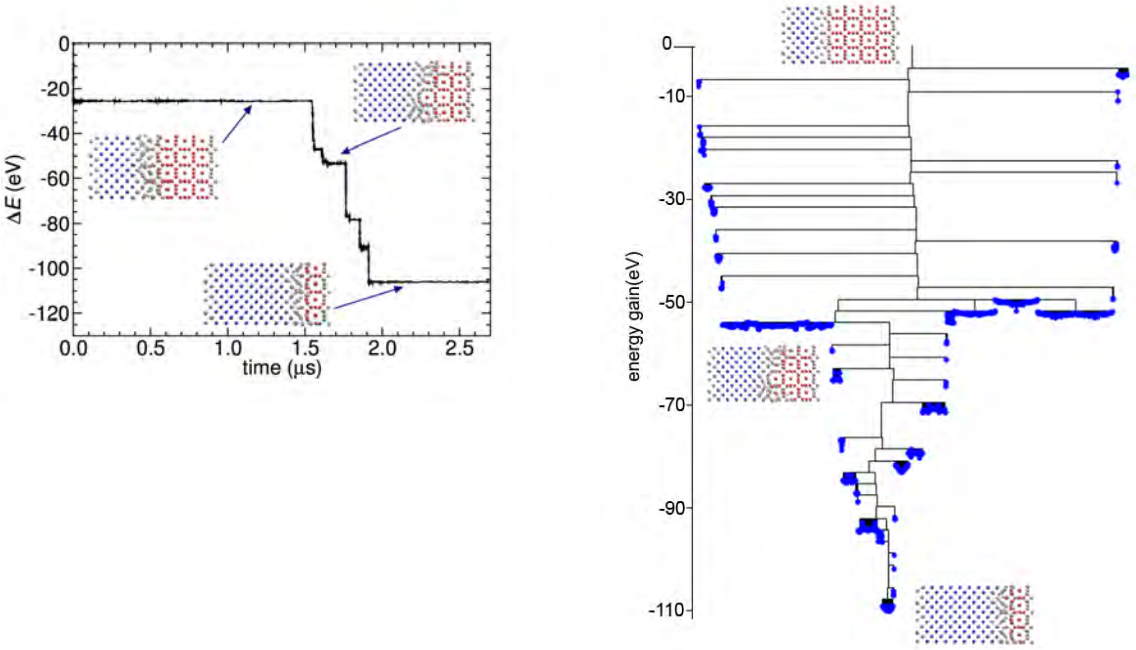
In this paper, we present the simulation of the eutectic phase transitions in the Pt–C system, in terms of both freezing and melting, using the multi-phase-field model. The experimentally obtained heat-extraction and -injection rates associated with the induction of freezing and melting are converted into the corresponding rates for microstructure-scale simulations. In spite of the extreme differences in the volume fractions of the FCC–Pt-rich phase on the one hand and graphite (C) on the other, satisfactory results for the kinetics of solidification and melting have been obtained, involving reasonable offsets in temperature, inducing freezing and melting, with respect to the equilibrium eutectic temperature. For freezing in the simulations, the needle/rod-like morphology, as experimentally observed, was reproduced for different heat extraction rates. The seemingly anomalous peak characterizing the simulated freezing curves is ascribed to the speed up of the solidification process due to the curvature effect. Similarly, a peak is observed in the experimental freezing curves, also showing up more clearly with increasing freezing rates. Melting was simulated starting from a frozen structure produced by a freezing simulation. The simulations reproduce the experimental melting curves and, together with the simulated freezing curves, help to understand the phase transition of the Pt–C eutectic. Finally, the effect of metallic impurities was studied. As shown for Au, impurities affect the morphology of the eutectic structure, their impact increasing with the impurity content, i.e., they can act as modifiers of the structure, as earlier reported for irregular eutectics.

2016

Collective atomic displacements during complex phase boundary migration in solid-solid phase transformations

J. Duncan, A. N. Harjunmaa, R. Terrell, R. Drautz, G. Henkelmann, J. Rogal

Physical Review Letters, **116**, 35701 (2016)



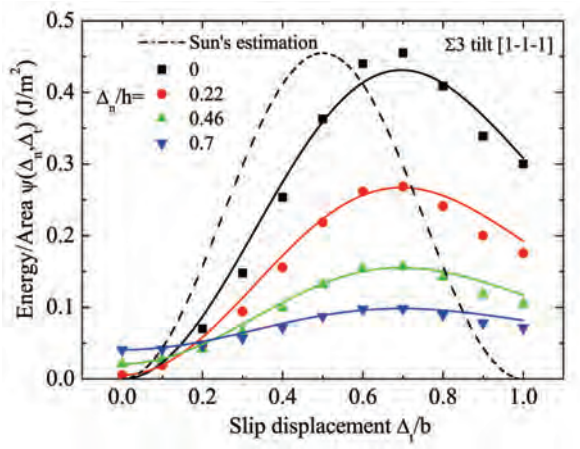
Left: Change in energy during the transformation from A15 to BCC in molybdenum along an adaptive kinetic Monte Carlo trajectory at T=300K. Right: Representation of the energy states that are visited along a trajectory in a disconnectivity graph.

The A15 to BCC phase transition is simulated at the atomic scale based on an interatomic potential for molybdenum. The migration of the phase boundary proceeds via long-range collective displacements of entire groups of atoms across the interface. To capture the kinetics of these complex atomic rearrangements over extended time scales, we use the adaptive kinetic Monte Carlo approach. An effective barrier of 0.5 eV is determined for the formation of each new BCC layer. This barrier is not associated with any particular atomistic process that governs the dynamics of the phase boundary migration. Instead, the effective layer transformation barrier represents a collective property of the complex potential energy surface.

Interplanar potential for tension-shear coupling at grain boundaries derived from ab initio calculations

X. Pang, R. Janisch, A. Hartmaier

Modelling and Simulation in Materials Science and Engineering, **24**, 15007 (2016)



Energy barrier for shear displacements of the Σ3(112) STGB in Al. Super-imposed tensile displacements lead to a flattening and a shift of the energy barrier, the so-called tension-softening effect. Symbols represent DFT data, lines the potential that is developed in the publication. Figure reprinted from MSMSE 24, 015007 (2016) under the terms of the Creative Commons Attribution 3.0 licence.

Based on ab initio density functional theory (DFT) calculations, we derive an analytical expression for the interplanar potential of grain boundaries and single crystals as a function of coupled tensile and shear displacements. This energy function even captures details of the grain boundary behaviour, such as the tension-softening of the shear instability of aluminium grain boundaries, with good accuracy. The good agreement between the analytical model and the DFT calculations is achieved by introducing two new characteristic parameters, namely the position of the generalised unstable stacking fault with respect to the stable stacking fault, and the ratio of stable and unstable generalised stacking fault energies. One of the potentials' parameters also serves as a criterion to judge if a grain boundary deforms via crack propagation or dislocation nucleation. We suggest this potential function for application in continuum models, where constitutive relationships for grain boundaries need to be derived from a sound physical model.

Complexity analysis of simulations with analytic bond-order potentials

C. Teijeiro Barjas, T. Hammerschmidt, B. Seiser, R. Drautz, G. Sutmann

Modelling and Simulation in Materials Science and Engineering, **24**, 25008 (2016)

The modelling of materials at the atomistic level with interatomic potentials requires a reliable description of different bonding situations and relevant system properties. For this purpose, analytic bond-order potentials (BOPs) provide a systematic and robust approximation to density functional theory (DFT) and tight binding (TB) calculations at reasonable computational cost. This paper presents a formal analysis of the computational complexity of analytic BOP simulations, based on a detailed assessment of the computationally most intensive parts. Different implementation algorithms are presented alongside optimizations for efficient numerical processing. The theoretical complexity study is complemented by systematic benchmarks of the scalability of the algorithms with increasing system size and accuracy level of the BOP approximation. Both approaches demonstrate that the computation of atomic forces in analytic BOPs can be performed with a similar scaling as the computation of atomic energies.

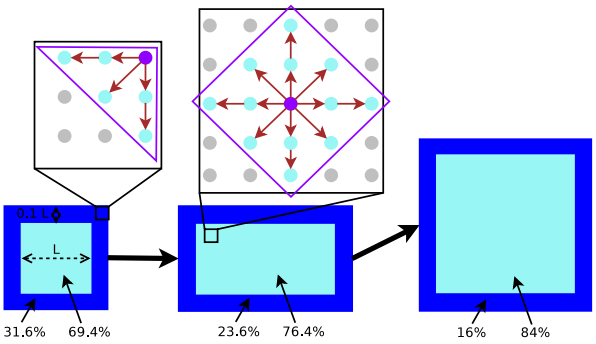


Illustration of computations that are required for analytic bond-order potentials for different fractions of bulk atoms and surface atoms in a two-dimensional sample system.

Crystal-structure analysis with moments of the density-of-states: Application to intermetallic topologically close-packed phases

T. Hammerschmidt, A. C. Ladines, J. Koßmann, R. Drautz

Crystals, **6**, 18 (2016)

$\Delta_{ij}^{(6)} \cdot 100$	bcc	χ	σ	A15	fcc	μ	C14	C36	C15
bcc	0.000	0.226	0.304	0.362	0.885	1.365	1.619	1.982	2.301
χ	-	0.000	0.220	0.315	0.808	1.301	1.550	1.922	2.247
σ	-	-	0.000	0.290	0.662	1.124	1.378	1.747	2.069
A15	-	-	-	0.000	0.818	1.161	1.403	1.769	2.091
fcc	-	-	-	-	0.000	0.655	0.886	1.236	1.546
μ	-	-	-	-	-	0.000	0.257	0.623	0.947
C14	-	-	-	-	-	-	0.000	0.375	0.702
C36	-	-	-	-	-	-	-	0.000	0.327
C15	-	-	-	-	-	-	-	-	0.000

Matrix of structural similarity of topologically close-packed phases ordered by increasing difference to bcc. The symmetric lower part is omitted for brevity.

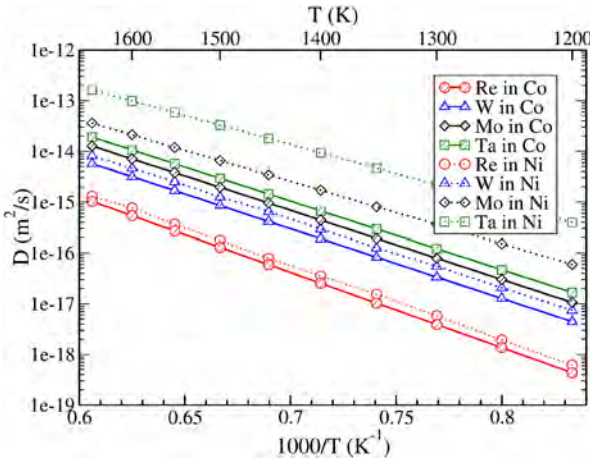
The moments of the electronic density-of-states provide a robust and transparent means for the characterization of crystal structures. Using d-valent canonical tight-binding, we compute the moments of the crystal structures of topologically close-packed (TCP) phases as obtained from density-functional theory (DFT) calculations. We apply the moments to establish a measure for the difference between two crystal structures and to characterize volume changes and internal relaxations. The second moment provides access to volume variations of the unit cell and of the atomic coordination polyhedra. Higher moments reveal changes in the longer-ranged coordination shells due to internal relaxations. Normalization of the higher moments leads to constant (A15, C15) or very similar (χ, C14, C36, μ, and σ) higher moments of the DFT-relaxed TCP phases across the 4d and 5d transition-metal series. The identification and analysis of internal relaxations is demonstrated for atomic-size differences in the V-Ta system and for different magnetic orderings in the C14-Fe_2Nb Laves phase.

Diffusion of solutes in FCC cobalt investigated by diffusion couples and first principles kinetic Monte Carlo

S. Neumeier, H. U. Rehman, J. Neuner, C. Zenk, S. Michel, S. Schuwalow, J. Rogal, R. Drautz, M. Göken

Acta Materialia, **106**, 304-312 (2016)

The interdiffusivity of Al and the transition metal solutes Ti, V, Cr, Mn, Fe, Nb, Mo, Ru, Ta, W, and Re in FCC Co is characterized at 1373 K, 1473 K and 1573 K by binary diffusion couples. The experimental results are complemented by first-principles calculations in combination with kinetic Monte Carlo simulations to investigate the diffusion of Re, W, Mo and Ta in FCC Co. The interdiffusion coefficients of alloying elements in FCC Co are generally smaller than in FCC Ni, but the correlation between interdiffusion coefficients and the atomic number of metal solutes is comparable in Co and Ni. With increasing atomic number and decreasing atomic radii, the interdiffusion coefficients of the investigated elements, except for Mn and Fe, decrease strongly. The trends in the diffusivity determined by experiment and simulation are in excellent agreement. Re is the slowest diffusing element in FCC Co among the investigated elements. The electronic structure calculations indicate that this is caused by strong directional bonds between Re and neighbouring Co atoms. The overall lower diffusivity of solute atoms in Co as compared to Ni suggests that diffusion controlled processes could be slower in Co-base superalloys.

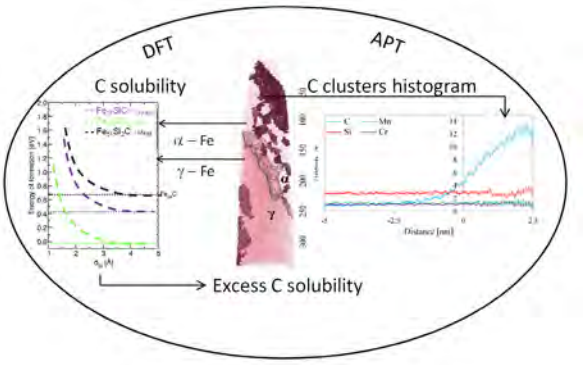


Comparison of diffusion coefficients of solute atoms Re, W, Mo and Ta in Ni and Co. The diffusion coefficients have been calculated using kinetic Monte Carlo simulations with input parameters from density-functional theory calculations.

The role of silicon, vacancies, and strain in carbon distribution in low temperature bainite

S. Sampath, R. Rementeria, X. Huang, J. D. Poplawsky, C. Garcia-Mateo, F. G. Caballero, R. Janisch

Journal of Alloys and Compounds, **673**, 289-294 (2016)



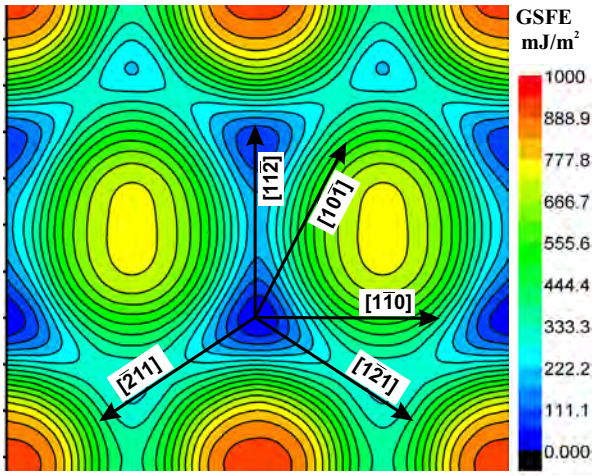
We compare the results of ab-initio calculations of carbon solubility with atom probe data to understand the influence of Si on the segregation of C in bainitic ferrite. Graphical abstract of Sampath et al., Journal of Alloys and Compounds 673, 289-294, 2016, reprinted with permission from Elsevier.

We investigated the phenomenon of carbon supersaturation and carbon clustering in bainitic ferrite with atom probe tomography (APT) and ab-initio density functional theory (DFT) calculations. The experimental results show a homogeneous distribution of silicon in the microstructure, which contains both ferrite and retained austenite. This distribution is mimicked well by the computational approach. In addition, an accumulation of C in certain regions of the bainitic ferrite with C concentrations up to 13 at % is observed. Based on the DFT results, these clusters are explained as strained, tetragonal regions in the ferritic bainite, in which the solution enthalpy of C can reach large, negative values. It seems that Si itself only has a minor influence on this phenomenon.

Stacking fault based analysis of shear mechanisms at interfaces in lamellar TiAl alloys

M. Kanani, A. Hartmaier, R. Janisch

Acta Materialia, **106**, 208-218 (2016)



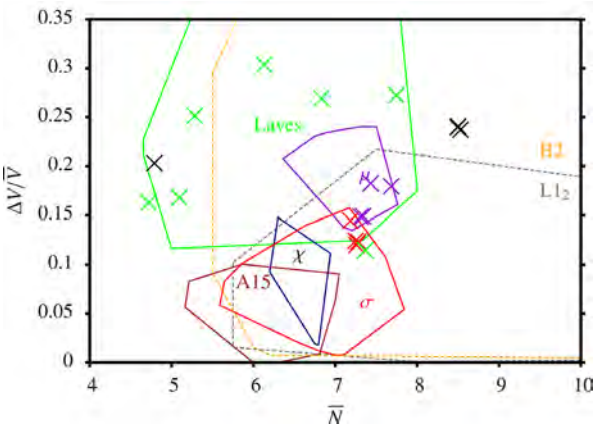
GSFE-surface of the (111) plane of a gamma-type single crystal. The main shearing directionsare indicated. Reprinted from Acta Mater. 106, 208-218 (2016) with permission from Elsevier.

The interfaces in lamellar TiAl alloys have a strong influence on the strength and deformability of the microstructure. It is widely accepted that their number and spacing can be used to tune these properties. However, the results of molecular dynamics simulations of sliding at g/g interfaces in lamellar TiAl alloys presented here suggest that important factors, namely the sequence of different interface types as well as the orientation of in-plane directions with respect to the loading axis, have to be included into meso-scale models. Simulations of bicrystal shear show significant differences in the deformation behaviour of the different interfaces, as well as pronounced in-plane anisotropy of the shear strength of the individual interfaces. The critical stresses derived from bicrystal shear simulations are of the same order of magnitude as the one for nucleation and motion of twins in a g-single crystal, showing that these mechanisms are competitive. In total, four different deformation mechanisms, interface migration, twin nucleation and migration, dislocation nucleation, and rigid grain boundary sliding are observed. Their occurrence can be understood based on a multilayer generalized stacking fault energy analysis. This link between physical properties, geometry, and deformation mechanism can provide guidelines for future alloy development.

The thermal stability of topologically close-packed phases in the single-crystal Ni-base superalloy ERBO/1

I. Lopez-Galilea, J. Koßmann, A. Kostka, R. Drautz, L. Mujica Roncery, T. Hammerschmidt, S. Huth, W. Theisen

Journal of Materials Science, **51**, 2653-2664 (2016)



Analysis of experimentally observed precipitates of topologically close-packed phases in heat-treated Ni-base superalloy ERBO1 in terms of a structure map using average number of valence electrons (N) and differences in atomic size (V). The crosses mark local chemical compositions of the precipitates obtained by TEM.

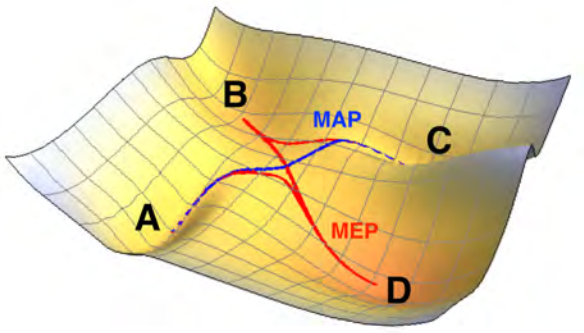
In Ni-base superalloys, the addition of refractory elements such as Cr, Mo, Co, W, and Re is necessary to increase the creep resistance. Nevertheless, these elements induce the formation of different kinds of intermetallic phases, namely, the topologically close-packed (TCP) phases. This work focuses on intermetallic phases present in the second-generation single-crystal (SX) Ni-base superalloy ERBO/1. In the as-cast condition, the typical γ/γ' structure is accompanied by undesirable intermetallic phases located in the interdendritic regions. The nature of these precipitates as well as their thermal stability between 800 and 1200 °C has been investigated by isothermal heat treatments. The investigation techniques include DSC, SEM, EDX, and TEM. The experimental information is complemented by (1) comparison with a structure map to link the local chemical composition with phase stability, as well as (2) thermodynamic calculations based on the CALPHAD method to determine the occurrence and composition of phases during solidification and in equilibrium conditions. The TCP phases Laves, μ and σ were identified in various temperature/time ranges.

Comparison of minimum-action and steepest-descent paths in gradient systems

G. Díaz Leines, J. Rogal

Physical Review E, **93**, 22307 (2016)

On high-dimensional and complex potential energy surfaces, the identification of the most likely mechanism for the transition between local minima is a challenging task. Usually the steepest-descent path is used interchangeably with the minimum-energy path and is associated with the most likely path. Here, we compare the meaning of the steepest-descent path in complex energy landscapes to the path integral formulation of a trajectory that minimizes the action functional for Brownian dynamics. In particular, for energy landscapes with bifurcation points and multiple minima and saddle points, there can be several steepest-descent paths associated with specific saddles that connect two predetermined states but largely differ from the path of maximum likelihood. The minimum-action path, however, additionally takes into account the scalar work along the trajectory. Minimizing the scalar work can be less ambiguous in the identification of the most likely path in different gradient systems. It can also be used to distinguish between multiple steepest-descent paths that connect reactant and product states. We illustrate that in systems with complex energy landscapes a careful assessment of the steepest-descent path is thus advisable. Here the evaluation of the action can provide valuable information on the analysis and description of the most likely path.

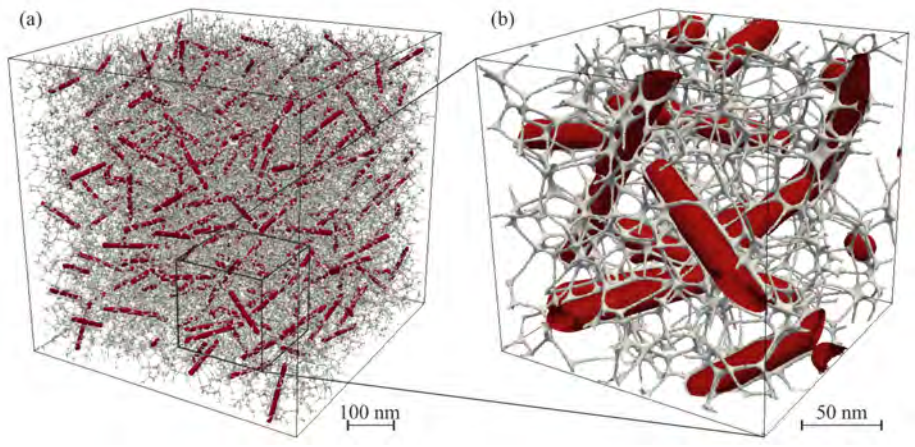


Minimum energy (MEP) and minimum action (MAP) paths on an asymmetric, four minima potential energy surface.

Phase-field study of Zener drag and pinning of cylindrical particles in polycrystalline materials

C. Schwarze, R. Darvishi Kamachali, I. Steinbach

Acta Materialia, 106, 59-65 (2016)



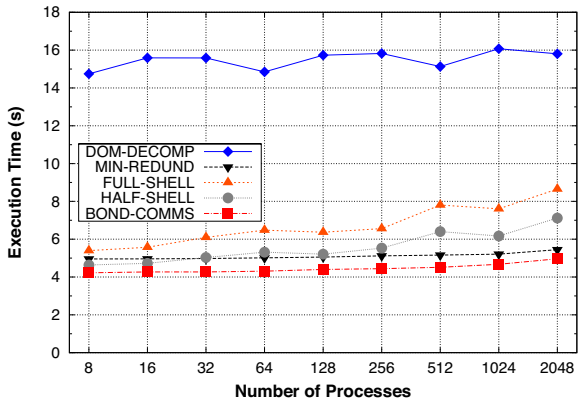
A systematic study of the secondary-phase particle pinning is conducted with a focus on the shape of the particles. The figure shows the large-scale simulation box with cylindrical particles and a zoom-in region. The network of grain boundaries surrounds the particles.

Zener drag and pinning in composites reinforced with cylindrical particles is investigated using three-dimensional phase-field simulations. Detailed systematic studies clarify the effect of relative orientation of the particle and length/diameter ratio on the kinetics of drag. It is shown that a combination of local equilibrium at junctions in contact with the particles, initial driving force of the migrating grain boundaries, and configuration of the particles within the polycrystalline matrix determine the intensity and persistence of drag and pinning effects.

Efficient parallelization of analytic bond-order potentials for large-scale atomistic simulations

C. Teijeiro Barjas, T. Hammerschmidt, R. Drautz, G. Sutmann

Computer Physics Communications, **204**, 64-73 (2016)



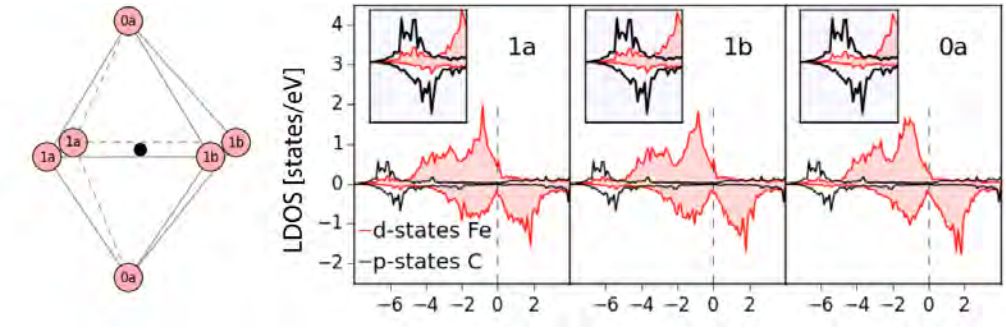
Comparison of weak scaling behaviour for different parallel implementations of analytic bond-order potentials. The implemented approaches differ by the ratio of redundancy and type of communication.

Analytic bond-order potentials (BOPs) provide a way to compute atomistic properties with controllable accuracy. For large-scale computations of heterogeneous compounds at the atomistic level, both the computational efficiency and memory demand of BOP implementations have to be optimized. Since the evaluation of BOPs is a local operation within a finite environment, the parallelization concepts known from short-range interacting particle simulations can be applied to improve the performance of these simulations. In this work, several efficient parallelization methods for BOPs that use three-dimensional domain decomposition schemes are described. The schemes are implemented into the bond-order potential code BOPfox, and their performance is measured in a series of benchmarks. Systems of up to several millions of atoms are simulated on a high performance computing system, and parallel scaling is demonstrated for up to thousands of processors.

First-principles study of carbon segregation in BCC iron symmetrical tilt grain boundaries

J. Wang, R. Janisch, G. Madsen, R. Drautz

Acta Materialia, **115**, 259-268 (2016)



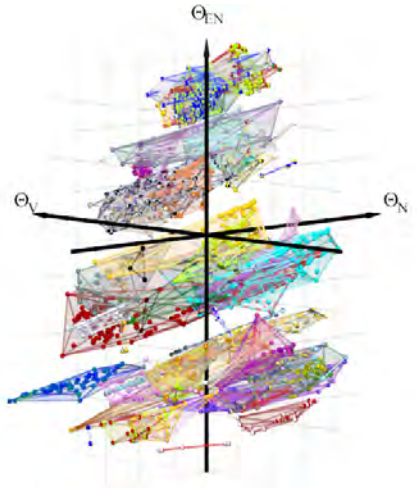
A carbon atom at the octahedral segregation site forms chemical bonds with surrounding iron atoms at the Σ3(112) grain boundary.

Segregation of light elements can profoundly affect the energies and cohesive properties of grain boundaries. First-principles calculations have been performed to determine the carbon solution energies and cohesive properties of three different grain boundaries in the presence of carbon. It is demonstrated that the most stable segregation sites possess the greatest coordination number and maximum Fe-C the nearest neighbour distance. Thereby, a geometric criterion for predicting the segregation sites is suggested. Open grain boundary structures are shown to be more attractive to C atoms than the compact grain boundary structure, vacancies and dislocations; and C segregation at open grain boundaries decreases the grain boundary energy. The theoretical fracture strength of grain boundaries increases with C concentration and tend to similar values for certain areal concentrations irrespective of the grain boundary structures. This implies that the maximum fracture strength of a grain boundary depends on the maximum C areal concentration it can accommodate.

Three-parameter crystal-structure prediction for sp-d-valent compounds

A. Bialon, T. Hammerschmidt, R. Drautz

Chemistry of Materials, **28**, 2550-2556 (2016)



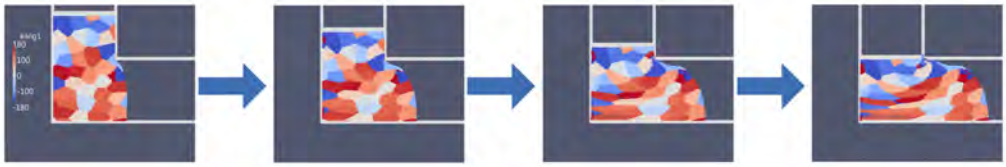
Three-dimensional map of structural stability of compounds formed by combining sp-valent elements with d-valent elements. The stability regions of the different crystal structures (polyhedrons) are spanned by descriptors that are based on atomic volume (V), number of electrons/holes (N) and electro-negativity (EN).

We present a three-dimensional structure map based on experimental data for compounds that contain sp-block elements and transition metals. The map predicts the correct crystal structure with a probability of 86% and has a confidence of more than 98% that the correct crystal structure is among three predicted crystal structures. The three descriptors of the structure map are physically intuitive functions of the number of valence electrons, atomic volume, and electronegativity of the constituent elements. We test the structure map against standard density-functional theory calculations for 1:1 sp-d-valent compounds and show that our three-parameter model has a comparable predictive power. We demonstrate the application of the structure map in conjunction with density-functional theory calculations.

A crystal plasticity smooth-particle hydrodynamics approach and its application to equalchannel angular pressing simulation

A. Ma, A. Hartmaier

Modelling and Simulation in Materials Science and Engineering, **24**, 085011 (2016)



Evolution of the microstructure during ECAP process as represented by the first Bunge Euler angle of the grains at 25%, 50%, 75% and 100% (from left to right). Graphic reprinted from Modelling and Simulation in Materials Science and Engineering, 24, 085011. © 2016 IOP Publishing. Reproduced with permission. All rights reserved.

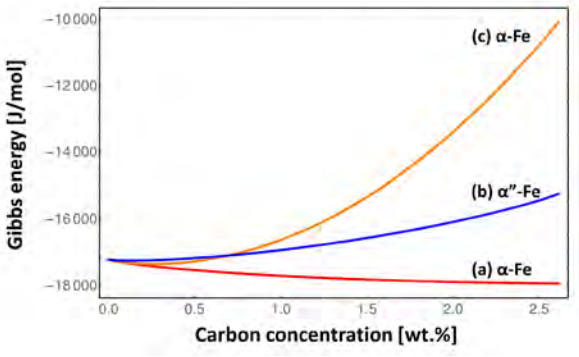
A crystal plasticity (CP) modelling approach based on smooth-particle hydrodynamics (SPH) has been developed to study severe plastic deformation of crystalline materials. The method has been implemented and validated by comparing the stress distribution and stress evolution of several SPH and FEM simulations for an anisotropic elastic material. The findings show that the SPH method produces an efficient and numerically robust solution for solid mechanics boundary value problems. Furthermore, the approach has been extended to incorporate a CP model and employed to simulate FCC polycrystals under the equal-channel angular pressing (ECAP) condition. It was found that the polycrystal contains four distinct regions with different deformation mechanisms. For the case that friction between deformable particles and boundary particles was neglected, more than one half of the grains suffered severe plastic deformation. The CP-SPH developed here thus proved to be a powerful tool to study grain refinement under severe plastic deformation.

Atomistically informed extended Gibbs energy description for phase-field simulation of tempering of martensitic steel

O. Shchyglo, T. Hammerschmidt, M. Cak, R. Drautz, I. Steinbach

Materials, **9**, 669 (2016)

In this study, we propose a unified multi-scale chemo-mechanical description of the BCT (Body-Centered Tetragonal) to BCC (Body-Centered Cubic) order-disorder transition in martensitic steel by adding the mechanical degrees of freedom to the standard CALPHAD (CALculation of PHAse Diagrams) type Gibbs energy description. The model takes into account external strain, the effect of carbon composition on the lattice parameter and elastic moduli. The carbon composition effect on the lattice parameters and elastic constants is described by a sublattice model with properties obtained from DFT (Density Functional Theory) calculations; the temperature dependence of the elasticity parameters is estimated from available experimental data. This formalism is crucial for studying the kinetics of martensite tempering in realistic microstructures. The obtained extended Gibbs energy description opens the way to phase-field simulations of tempering of martensitic steel comprising microstructure evolution, carbon diffusion and lattice symmetry change due to the ordering/disordering of carbon atoms under multiaxial load.

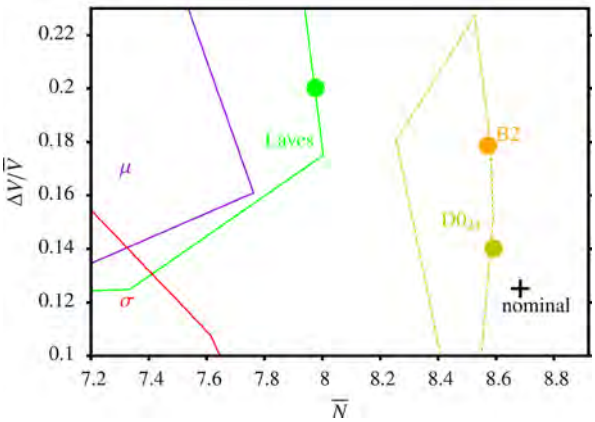


Gibbs energies: (a) α-Fe without chemomechanical coupling, (b) α-Fe reference configuration and (c) α-Fe considering chemomechanical coupling effect. The difference between the curves (a) and (c) indicates significant phase stability change if chemomechanical coupling effect is considered.

The role of local chemical composition for TCP phase precipitation in Ni-base and Co-base superalloys

T. Hammerschmidt, J. Koßmann, C. Zenk, S. Neumeier, M. Göken, I. Lopez-Galilea, L. Mujica, S. Huth, A. Kostka, W. Theisen, R. Drautz

Superalloys 2016: Proceedings of the 13th International Symposium on Superalloys, 89-96 (2016)



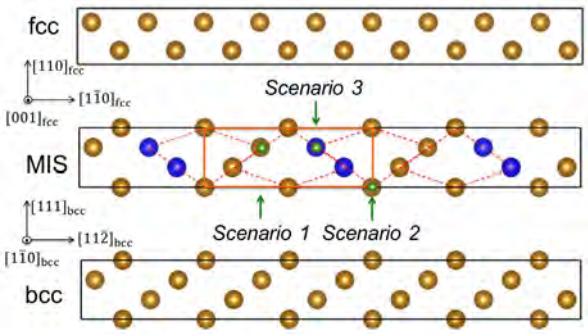
Analysis of experimentally observed precipitates in as-cast Ni-base superalloy ERBO-Co0 in terms of a structure map using average number of valence electrons (N) and differences in atomic size (V). The circles mark local chemical compositions obtained by TEM.

The precipitation of topologically close-packed (TCP) phases in single-crystal superalloys is highly undesirable due to the detrimental effect on the mechanical properties. The TCP phases bind atoms responsible for the solid solution strengthening of the γ phase (Re, W, Mo), as well as elements that are important for the formation of the γ' phase (Ti, Ta). A thorough understanding of TCP phase precipitation is therefore a prerequisite for the design of future superalloys. The thermodynamic stability of TCP phases as bulk material is well understood, but little is known about the factors that govern the stability of the experimentally observed precipitates of TCP phases within the superalloy matrix. The focus of this paper is on the role of the local chemical composition for the stability of TCP phase precipitates. We combine experimental measurements of the local chemical composition of TCP phase precipitates in the Ni-base superalloy ERBO-1 and the Co-base superalloy ERBO-Co0 with a theory-guided interpretation of the structural stability of bulk TCP phases. The experimental characterization of the microstructure and the crystal structure of the precipitates are based on scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The local chemical composition is determined by energy-dispersive X-ray spectroscopy (EDX) and electron probe microanalysis (EPMA). The measured local chemical compositions are assessed regarding the likelihood of TCP phase formation by determining their location in a structure map of the stability of bulk TCP phases. This establishes a direct link between the measured local chemical composition of TCP phase precipitates and the phase stability of bulk TCP phases at this composition. By converting the measured local chemical composition into structure map coordinates, we effectively construct a compound map that indicates the regions in the microstructure that are prone to TCP phase precipitation. Analyzing the intermetallic precipitates in more detail, we find that the chemical compositions of the TCP phase precipitates would be expected to form the same TCP phase as bulk material. This suggests that the observed precipitates of TCP phases can be regarded to be in a local thermodynamic equilibrium. The challenge of predicting TCP phase precipitation in superalloys is hence reduced to the prediction of the local chemical composition during casting, heat treatment and service.

Interplay between interstitial displacement and displacive lattice transformations

X. Zhang, T. Hickel, J. Rogal, J. Neugebauer

Physical Review B, **94**, 104109 (2016)



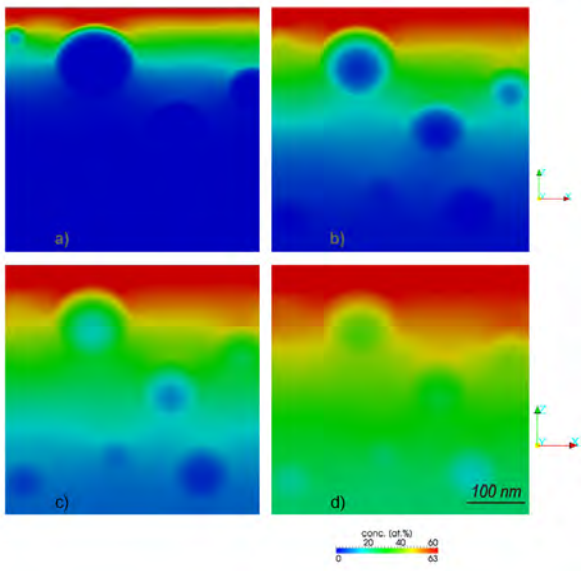
Three scenarios for C redistribution during the transformation from FCC via the metastable intermediate structure (MIS) into BCC Fe. The transformation from the (MIS) involves mainly an atomic shuffle of the corresponding Fe atoms (blue spheres) along the $[111]_{bcc}$ direction. Green, small spheres indicate C atoms.

Diffusionless displacive lattice rearrangements, which include martensitic transformations, are in real materials often accompanied by a displacive drag of interstitials. The interplay of both processes leads to a particular atomistic arrangement of the interstitials in the product phase, which is decisive for its performance. An archetype example is the martensitic transformation in Fe-C alloys. One of the puzzles for this system is that the deviation from the cubic symmetry (i.e., the tetragonality) in the martensite resulting from this interplay is lower than what thermodynamics dictates. In our ab initio approach, the relative motion of C in the transforming lattice is studied with the nudged elastic band method. We prove that an atomic shearlike shuffle mechanism of adjacent $(11\bar{2})$ Fe layers along the $\pm[111]_{bcc}$ directions is essential to achieve a redistribution of C atoms during the FCC -> BCC transition, which fully explains the abnormal behaviour. Furthermore, the good agreement with experimental data validates our method to treat a diffusionless redistribution of interstitials and a displacive rearrangement of the host lattice simultaneously.

Phase field modelling of intercalation kinetics: A finite interface dissipation approach

N. Alemayehu, I. Steinbach

MRS Communications, **6**, 270-282 (2016)



Lithium concentration during intercalation in an arrangement of active $FePO_4$ particles embedded in electrolyte. From a) to d) different time steps up to 32 ns are shown. The colour scale is Li concentration between 0% (blue) and 60% (red).

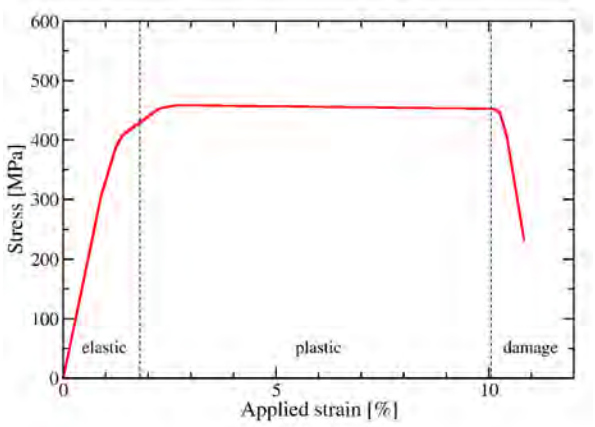
When two materials interact, the processes between the phases determine the functional properties of the compound. Pivotal interface phenomena are diffusion and redistribution of atoms (molecules). This is especially of interest in Lithium-ion batteries, where the interfacial kinetics determine the battery performance and impact cycling stability. A new phase-field model, which links the atomistic processes at the interface to the mesoscale transport by a redistribution flux controlled by the so called 'interface permeability' was developed. The model was validated with experimental data from diffusion couples. Calculations of the concentration profiles of the species at the electrode–electrolyte interface are reported. Active particle size, morphology and spatial arrangement were put into correlation with diffusion behaviour for use in reverse engineering.

Full-field simulation of solidification and forming of polycrystals

E. Borukhovich, M. Boeff, A. Monas, M. Tegeler, S. Kim, C. Oh, I. Steinbach

MATEC Web of Conferences, **80**, 2014 (2016)

The phase-field method has emerged as the method of choice for the simulation of microstructure evolution and phase-transformations in materials science. It has wide applications in solidification and solid state transformations in general. Recently, the method has been generalized to treat large deformation and damage in solids. A through-process full-field simulation will be presented starting from solidification and ending with the evolution of damage during large deformation. Aspects of numerical discretization, efficient numerical integration and massive parallelization will be discussed.



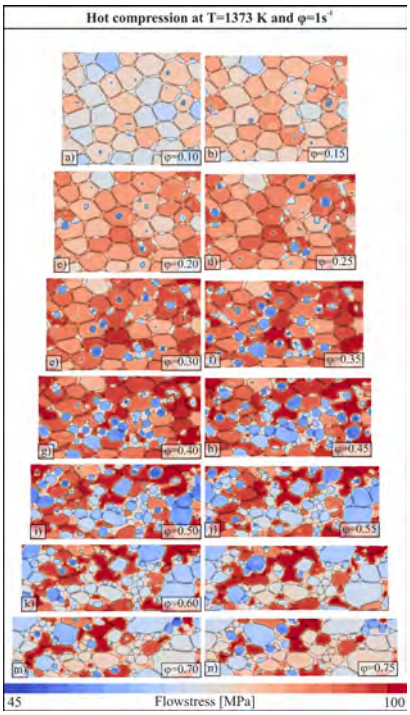
Stress-Strain curve as result of the virtual tensile testing of the simulated solidified Mg-5%Al microstructure. Both simulations are performed within the OpenPhase framework.

Modelling of flow behaviour and dynamic recrystallization during hot deformation of MS-W 1200 using the phase-field framework

J. Hiebeler, K. Khlopkov, O. Shchyglo, T. Pretorius, I. Steinbach

MATEC Web of Conferences **80**, 01003 (2016) NUMIFORM 2016, **80**, 1003 (2016)

A new simulation environment is developed to simulate the evolution of microstructure and the corresponding flow stress during rolling. An orientation dependent crystal plasticity hardening model is coupled to grain evolution-, recovery- and recrystallization kinetics within a phase-field framework. Hardening and softening kinetics are treated consecutively to differentiate between individual effects. Simulation results are compared to hot compression tests at 1373 K with a strain rate of 1 s^{-1}.

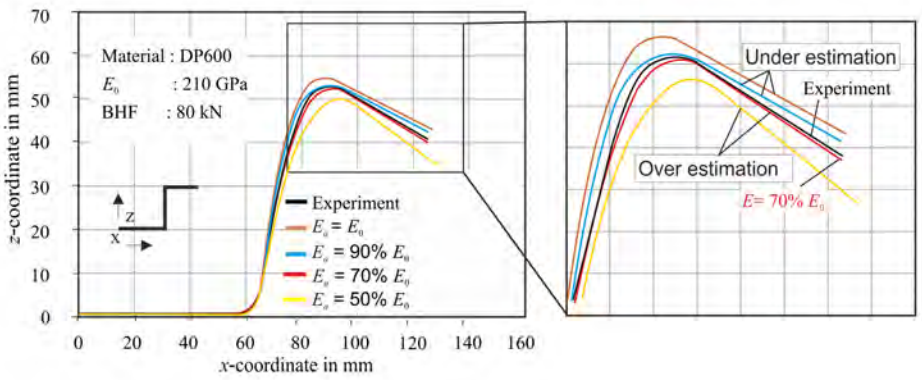


Microstructure evolution during hot deformation of MS-W 1200 steel at 1373 K and strain rate of 1/s. Colour coding gives flow stress in [MPa].

Springback prediction and reduction in deep drawing under influence of unloading modulus degradation

H. u. Hassan, F. Maqbool, A. Güner, A. Hartmaier, N. Ben Khalifa, E. Tekkaya

International Journal of Material Forming, **9**, 619-633 (2016)



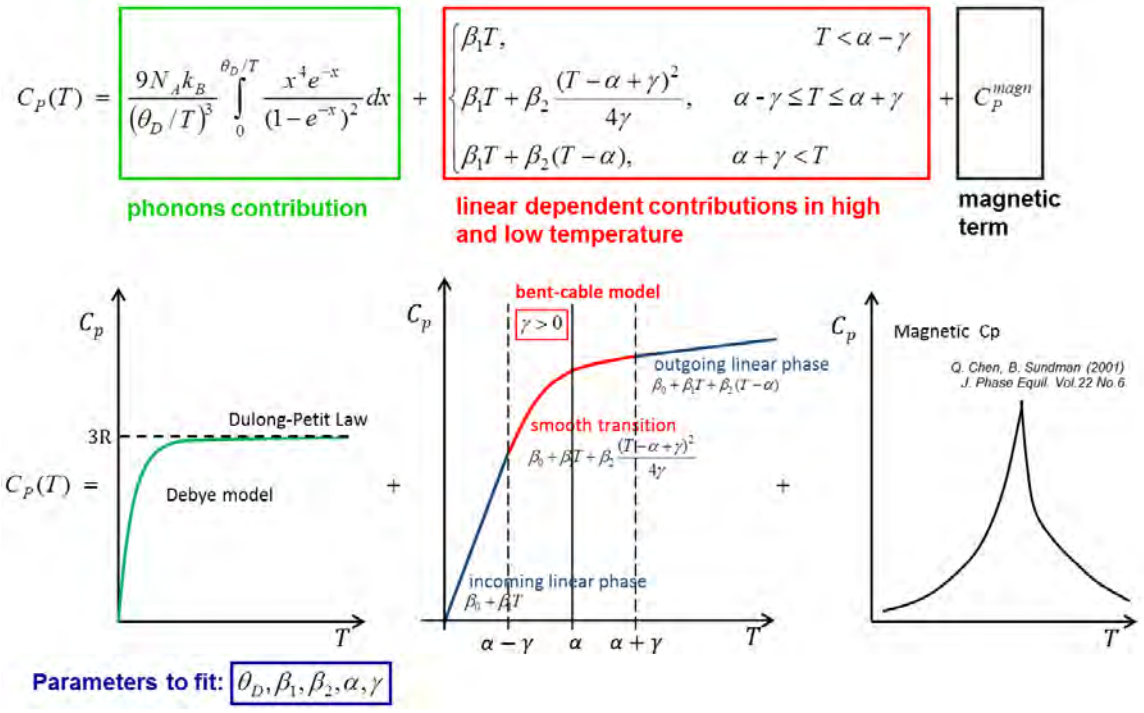
Effect of Young´s modulus degradation on the springback prediction.

Springback is considered as one of the major problems in deep drawing of high-strength steels (HSS) and advanced high-strength steels (AHSS) which occurs during the unloading of part from the tools. With an ever increasing demand for the production of lightweight automobile structures and increased crash performance, the use of HSS and AHSS is becoming extensive. For the accurate prediction of springback, unloading behaviour of dual phase steels DP600, DP1000 and cold rolled steel DC04 for the deep drawing process is investigated and a strategy for the reduction of springback based on variable blankholder force is also presented. Cyclic tension compression tests and LS-Opt software are used for the identification of material parameters for the Yoshida-Uemori (YU) model. Degradation of the Young's modulus is found to be 28 and 26 and 14 % from the initial Young's modulus for DP600, DP1000 and for the DC04 respectively for the saturated value. A finite element model is generated in LS-DYNA based on the kinematic hardening material model Yoshida-Uemori (YU). The validation of numerical simulations is also carried out by the real deep drawing experiments. Springback could be predicted with the maximum deviation of 1.1 mm for these materials. For DP1000, the maximum springback is reduced by 24.5 %, for DP600 33.3 and 48.7 % for DC04 by the application of monotonic blankholder force instead of a constant blankholder force of 80 kN. It is concluded that despite the reduction of Young's modulus, the springback for these materials can be reduced by increasing the blankholder force only in the last 13 % of the punch travel.

Modelling of Gibbs energies of pure elements down to 0 K using segmented regression

I. Roslyakova, B. Sundman, H. Dette, L. Zhang, I. Steinbach

CALPHAD Journal, **55**, 165-180 (2016)



Segmented regression model for the heat capacity of solids.

A novel thermodynamic modelling strategy of stable solid alloy phases is proposed based on a segmented regression approach. The model considers several physical effects (e.g. electronic, vibrational, etc.) and is valid from 0 K up to the melting temperature. The preceding approach has been applied for several pure elements. Results show good agreement with experimental data at low and high temperatures. Since this is not the first attempt to propose a "universal" physics-based model down to 0 K for the pure elements as an alternative to current SGTE description, we also compare the results to existing models. Analysis of the obtained results shows that the newly proposed model delivers more accurate description down to 0 K for all studied pure elements, according to several statistical tests.

ICAMS Members 2015 and 2016

13. ICAMS Members 2015 and 2016

Staff at ICAMS

About 70-80 researchers, including PhD students, work at ICAMS; about 5 administrative staff and 4 technicians. support the institute. Since the end of the start up funding in 2013, staff numbers decreased by about 15%, largely due to a smaller number of industry projects.

Fig. 13.1 shows the development of ICAMS staff numbers through the first nine years. By the end of 2008 about 30 people were working at ICAMS. From 2009 to 2013 this number increased to more than 80, and by the end of 2014 almost 90 people worked at ICAMS. In 2016 ICAMS' staff numbers have decreased to the level of 2012.

The majority of ICAMS scientists hold a degree in engineering and materials science, followed by degrees in physics, mathematics or computer science and chemistry (*Fig. 13.2*). This educational diversity of our research staff provides the basis for ICAMS' interdisciplinary research.

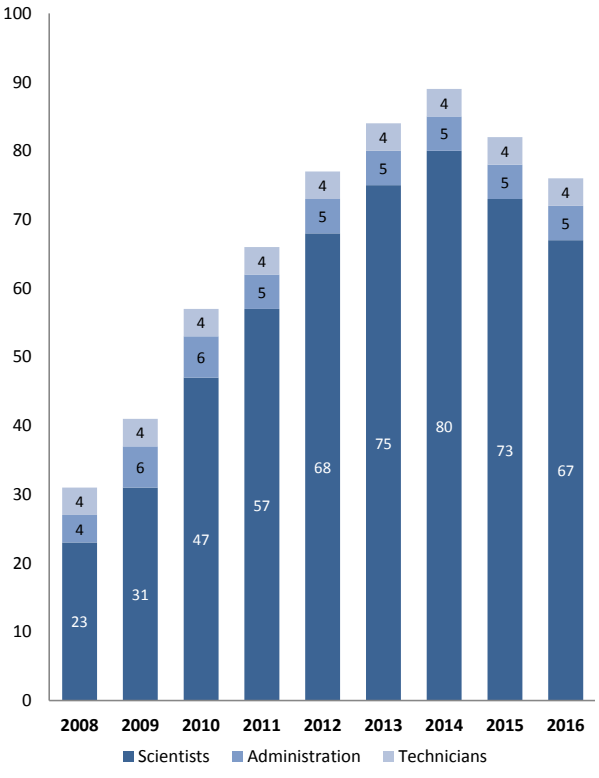


Fig. 13.1: Development of ICAMS staff from 2008 to 2016.

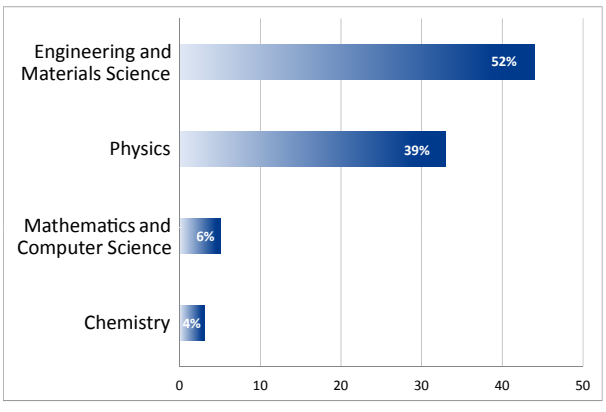
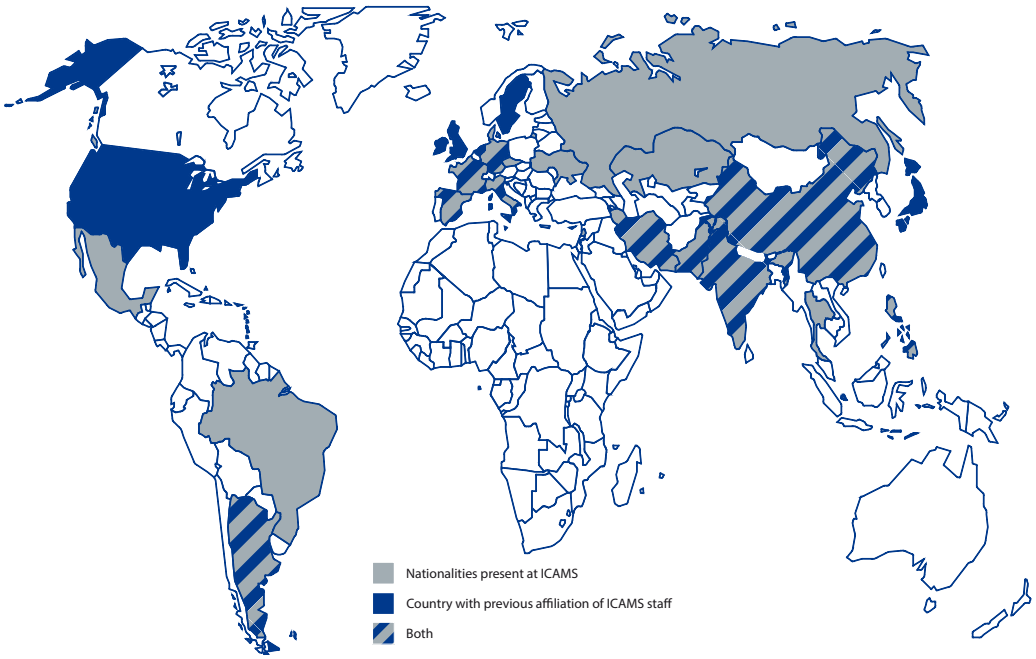


Fig. 13.2: Breakdown of first degree of ICAMS researchers.

In 2015 and 2016 researchers from 18 different countries were working at ICAMS (see grey areas in *Fig. 13.3*). 42% of the ICAMS staff is of German and 58% of foreign nationality. For ICAMS, it is of vital importance to attract talented scientists from leading research institutions worldwide. *Fig. 3* gives an overview of the countries and institutions of origin of the current ICAMS researchers. 12 of the 50 institutions are located in Germany, 14 in other EU countries and 24 in non-EU countries. Staff members are encouraged to stay in contact with their previous research institutions, thus helping ICAMS to establish a tight network of international collaborations.



Previous affiliations of ICAMS members

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Chinese Academy of Sciences, Shenyang
Northwestern Polytechnical Univ., Xi'an Shaanxi

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Aarhus University

France
LEM-ONERA-CNRS, Chatillion
INSA Lyon
Université de Metz
CNRS, Paris

Germany
AICE, Aachen
RWTH Aachen
Ruhr-Universität Bochum
TU Dortmund
MPI für Eisenforschung, Düsseldorf
Friedrich-Alexander Univ., Erlangen-Nürnberg
Goethe-Universität, Frankfurt am Main
Fraunhofer IWM, Freiburg
Universität Hamburg
Forschungszentrum Jülich
BASF, Ludwigshafen
Bergische Universität Wuppertal

India
Anna University, Chennai
Larson & Toubro Limited, Chennai
Indian Institute of Technology, Guwahati
JNTU Heiderabad
Indian Institute of Technology, Mumbai
Pondicherry University
University of Pune

Iran
University of Guilan, Rasht
University of Advanced Technology, Kerman
Sahand University of Technology
Shiraz University
Amirkabir University of Technology, Teheran
K. N. Toosi University of Technology, Teheran

Ireland
Trinity College, Dublin

Italy
NNL of CNR-INFM, Lecce
University of Trento
University of Trieste

Japan
University of Tokio
National Institute for Materials Science, Tsukuba

The Netherlands
University of Amsterdam

Pakistan
University of Engineering & Technology, Lahore
Ghulam Ishaq Khan Institute of Engineering Sciences and Technology, Topi

Philippines
De La Salle University, Manila

Spain
University of la Coruna

Sweden
University of Linköping

United Kingdom
University of Oxford
Imperial College, London

USA
University of Pennsylvania, Philadelphia (PA)

Fig. 13.3: Nationalities at ICAMS. The countries of origin of ICAMS staff are highlighted in grey, the countries with previous affiliations of ICAMS members are marked in blue, and the countries where both criteria are met are marked in grey-blue stripes. The previous affiliations of ICAMS staff members are listed.

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Zinn, Arndt-Hendrik, M.Sc.
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External
(at ICAMS until April 2015)

Publications

14. Publications

>> Proceedings and other publications 2015

C. Teijeiro Barjas, T. Hammerschmidt, R. Drautz, G. Sutmann
Parallel bond order potentials for materials science simulations
Proceedings of the 4th International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering (2015) 4

M. Tegeler, A. Monas, G. Sutmann
Massively parallel multiphase field simulations
Proceedings of the 4th International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering (2015) 5

A. Monas, O. Shchyglo, D. Höche, M. Tegeler, I. Steinbach
Dual-scale phase-field simulation of Mg-Al alloy solidification
IOP Conference Series Materials Science and Engineering, 84 (2015) 012069

>> Proceedings and other publications 2016

V. Kulitskiy, S. Malopheyev, Y. Buranova, S. V. Divinski, G. Wilde, R. Kaibyshev
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T. Hammerschmidt, J. Koßmann, C. Zenk, S. Neumeier, M. Göken, I. Lopez-Galilea, L. Mujica, S. Huth, A. Kostka, W. Theisen, R. Drautz
The role of local chemical composition for TCP phase precipitation in Ni-base and Co-base superalloys
Superalloys 2016: Proceedings of the 13th International Symposium on Superalloys (2016) 89-96

C. Zenk, S. Neumeier, M. Kolb, N. Volz, S. G. Fries, O. Dolotko, I. Povstugar, D. Raabe, M. Göken
The role of the base element in γ-strengthened cobalt/nickel-base superalloys
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Modelling of flow behaviour and dynamic recrystallization during hot deformation of MS-W 1200 using the phase field framework
MATEC Web of Conferences (2016) 1003

E. Borukhovich, M. Boeff, A. Monas, M. Tegeler, S. Kim, C. Oh, I. Steinbach
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>> Publications in refereed journals 2015

L. Morales-Rivas, V. Yardley, C. Capdevila, C. Garcia-Mateo, H. Roelofs, F. G. Caballero
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Journal of Materials Science, 50 (2015) 258-267

A. Ma, A. Hartmaier
A study of deformation and phase transformation coupling for TRIP-assisted steels
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B. Sundman, U. R. Kattner, M. Palumbo, S. G. Fries
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Integrating Materials and Manufacturing Innovation, 4 (2015) 1

B. Sundman, M. Stratmann, L. Zhang, Y. Du
Computational thermodynamics and its applications in materials science
Materials China, 34 (2015) 15-29

C. Begau, G. Sutmann
Adaptive dynamic load-balancing with irregular domain decomposition for particle simulations
Computer Physics Communications, 190 (2015) 51-61

P. Wollgramm, H. Buck, K. Neuking, A. B. Parsa, S. Schuwalow, J. Rogal, R. Drautz, G. Eggeler
On the role of Re in the stress and temperature dependence of creep of Ni-base single crystal superalloys
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Acta Materialia, 99 (2015) 281-289

A. Katre, A. Togo, I. Tanaka, G. Madsen
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Journal of Applied Physics, 117 (2015) 045102

S. V. Divinski, G. Reglitz, I. S. Golovin, M. Peterlechner, R. Lapovok, Y. Estrin, G. Wilde
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Surface Science, 631 (2015) 190-195

X. Chen, C. Si, Y. Gao, J. Frenzel, J. Sun, G. Eggeler, Z. Zhang
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Journal of Power Sources, 273 (2015) 324-332

B. Ziebarth, M. Mrovec, C. Elsässer, P. Gumbsch
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Acta Materialia, 88 (2015) 156-169

J. Gehrmann, D. G. Pettifor, A. Kolmogorov, M. Reese, M. Mrovec, C. Elsässer, R. Drautz
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Journal of Physics: Condensed Matter, 27 (2015) 086002

P. Nörtershäuser, J. Frenzel, A. Ludwig, K. Neuking, G. Eggeler
The effect of cast microstructure and crystallography on rafting, dislocation plasticity and creep anisotropy of single crystal Ni-base superalloys
Materials Science and Engineering A, 626 (2015) 305-312

S. G. Ayodele, D. Raabe, F. Varnik
Shear-flow-controlled mode selection in a nonlinear autocatalytic medium
Physical Review E, 91 (2015) 022913

D. Belardinelli, M. Sbragaglia, L. Biferale, M. Gross, F. Varnik
Fluctuating multicomponent lattice Boltzmann model
Physical Review E, 91 (2015) 023313

M. Gross, T. Krüger, F. Varnik
Fluctuations and diffusion in sheared athermal suspensions of deformable particles
Europhysics Letters, 108 (2015) 68006

M. Q. Jiang, G. Wilde, L. H. Dai
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Mechanics of Materials, 81 (2015) 72-83

D. C. Ma, D. Raabe, M. Friák, J. von Pezold, J. Neugebauer
Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation
Acta Materialia, 85 (2015) 53-66

X. Yan, H. Xiong, Q. Bai, J. Frenzel, C. Si, X. Chen, G. Eggeler, Z. Zhang
Atomic layer-by-layer construction of Pd on nanoporous gold via underpotential deposition and displacement reaction
RSC Advances, 5 (2015) 19409-19417

S. Gao, M. Fivel, A. Ma, A. Hartmaier
Influence of misfit stresses on dislocation glide in single crystal superalloys: A three-dimensional discrete dislocation dynamics study
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T. Chakraborty, J. Rogal, R. Drautz
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Journal of Physics: Condensed Matter, 27 (2015) 115401

W. Kochański, M. Boeff, Z. Hashemiyan, W. J. Staszewski, P. K. Verma
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Journal of Sensors, 2015 (2015) 796439

S. Bhattacharya, N. S. Gunda, R. Stern, S. Jacobs, R. Chmielowski, G. Dennler, G. Madsen
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Physical Chemistry Chemical Physics, 17 (2015) 9161-9166

R. Chmielowski, D. Pere, C. Bera, I. Opahle, W. Xie, S. Jacob, F. Capet, P. Roussel, A. Weidenkaff, G. Madsen
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C. Simon, M. Peterlechner, G. Wilde
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A. C. Ladines, T. Hammerschmidt, R. Drautz
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S. Gupta, A. Ma, A. Hartmaier
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J. Frenzel, A. Wieczorek, I. Opahle, B. Maaß, R. Drautz, G. Eggeler
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R. Darvishi Kamachali, A. Abbondandolo, K. F. Siburg, I. Steinbach
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T. Chakraborty, A. Hens, S. Kulashrestha, N. C. Murmu, P. Banerjee
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J. Zhang, C. Begau, L. Geng, A. Hartmaier
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Wear, 332-333 (2015) 941-948

J. Buenz, K. A. Padmanabhan, G. Wilde
On the applicability of a mesoscopic interface sliding controlled model for understanding superplastic flow in bulk metallic glasses
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Y. P. Mitrofanov, M. Peterlechner, I. Binkowski, M. Y. Zadorozhnyy, I. S. Golovin, S. V. Divinski, G. Wilde
The impact of elastic and plastic strain on relaxation and crystallization of Pd–Ni–P-based bulk metallic glasses
Acta Materialia, 90 (2015) 318-329

D. Prokoshkina, L. Klinger, A. Moros, G. Wilde, E. Rabkin, S. V. Divinski
Persistence of ultrafast atomic diffusion paths in recrystallizing ultrafine grained Ni
Scripta Materialia, 101 (2015) 91-94

B. Dutta, T. Hickel, J. Neugebauer, C. Behler, S. Fähler, A. Behler, A. Waske, N. Teichert, J. M. Schmalhorst, A. Hütten
Interplay of strain and interdiffusion in Heusler alloy bilayers
Physica Status Solidi RRL, 9 (2015) 321-325

K. D. Bauer, M. Todorova, K. Hingerl, J. Neugebauer
A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron
Acta Materialia, 90 (2015) 69-76

G. Leyson, B. Grabowski, J. Neugebauer
Multiscale description of dislocation induced nano-hydrides
Acta Materialia, 89 (2015) 50-59

A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer
Understanding anharmonicity in the fcc materials: From its origin to ab initio strategies beyond the quasiharmonic approximation
Physical Review Letters, 114 (2015) 195901

B. Grabowski, A. Glensk, T. Hickel, J. Neugebauer
Random phase approximation up to the melting point: Impact of anharmonicity and nonlocal many-body effects on the thermodynamics of Au
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R. Darvishi Kamachali, S. Kim, I. Steinbach
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S. Gupta
Micromechanical modeling of martensitic phase transformation in steels based on nonlocal crystal plasticity
PhD Thesis, Ruhr-Universität Bochum (2015)

A. C. Ladines
Influence of light elements on precipitates of complex phases in steel
PhD Thesis, Ruhr-Universität Bochum (2015)

A. Katre
Modelling thermal transport in nanostructured materials
PhD Thesis, Ruhr-Universität Bochum (2015)

A. A. Gießmann
The influence of stress enhanced diffusion on the growth of pearlite in eutectoid plain carbon steel
PhD Thesis, Ruhr-Universität Bochum (2015)

M. Kanani
Correlation of deformation mechanisms and atomistic structure of interfaces in lamellar TiAl alloys
PhD Thesis, Ruhr-Universität Bochum (2015)

S. Kenmoe
Ab initio study of the low-index non-polar zinc oxide surfaces in contact with water: From single molecules to multilayers
PhD Thesis, Ruhr-Universität Bochum (2015)

P. Schwittek
Micromechanical and continuum modeling of hydrogen assisted steel degradation
PhD Thesis, Ruhr-Universität Bochum (2015)

T. Wang
Large-scale molecular dynamics simulation of growth, microstructure and properties of thermal-sprayed coatings
PhD Thesis, Ruhr-Universität Bochum (2015)

X. Zhang
Structural transformations in Fe-C alloys: From atomistic simulations to a microscopic understanding
PhD Thesis, Ruhr-Universität Bochum (2015)

E. Borukhovich
Consistent coupling of geometrically non-linear finite deformation with alloy chemistry and diffusion within the phase-field framework
PhD Thesis, Ruhr-Universität Bochum (2015)

D. Yan
Micromechanically guided design of graded ultra-fine-grained dual-phase steel
PhD Thesis, Ruhr-Universität Bochum (2015)

A. Hariri
Phase transitions in high manganese steels: Simulation and experiment
Master Thesis, Ruhr-Universität Bochum (2015)

U. V. Unije
Simulation of transport processes through asymmetric gas separation membrane
Master Thesis, Ruhr-Universität Bochum (2015)

A. Wengert
Initial stages of internal oxidation of iron base alloys in the temperature range of 600°C to 850°C
Master Thesis, Ruhr-Universität Bochum (2015)

L. Sharma
Implementation and comparison of different damage criteria in the framework of crystal plasticity
Master Thesis, Ruhr-Universität Bochum (2015)

A. Lange
Ti-Ta based high-temperature shape memory alloy thin films
Master Thesis, Ruhr-Universität Bochum (2015)

N. Rivas
Sulfidation resistance of Ni-Cr alloys exposed to simulated coal power plant atmospheres
Master Thesis, Ruhr-Universität Bochum (2015)

M. Heyn
Evolution of the grain boundary microstructure on tempering of a 2.25Cr1Mo steel
Master Thesis, Ruhr-Universität Bochum (2015)

A. Kauws
Investigation of mechanical properties of martensite packets using inverse analysis
Master Thesis, Ruhr-Universität Bochum (2015)

A. Gupta
Precipitation kinetics in binary alloys
Master Thesis, Ruhr-Universität Bochum (2015)

S. Ramesh Babu
Additive manufacturing of nickel-base superalloys: A phase-field study
Master Thesis, Ruhr-Universität Bochum (2015)

M. M. Golam
Investigation of hydrogen trapping in model alloys with and without internal oxide precipitates
Master Thesis, Ruhr-Universität Bochum (2015)

H. Shabbir
Multi scale simulations: Interaction between γ' precipitate and interfacial dislocation in nickel base superalloys
Master Thesis, Ruhr-Universität Bochum (2015)

B. Dongre
The effect of a vacancy on the thermal conductivity of Stillinger-Weber silicon
Master Thesis, Ruhr-Universität Bochum (2015)

C. Park
DFT+U calculations of delithiation at Σ2 tilt grain boundary in $Li[Co_{1/3}Ni_{1/3}Mn_{1/3}]O_2$ cathode material for Lithium-ion battery
Master Thesis, Ruhr-Universität Bochum (2015)

U. Kaya
Development of simulation methods for characterization and modeling of tribological properties of thin metal sheets
Master Thesis, Ruhr-Universität Bochum (2015)

A. K. Kothapalli
RVE based characterization and homogenization of elasto plastic properties for woven thermoplastic composite materials
Master Thesis, Ruhr-Universität Bochum (2015)

L. Poggenpohl
Entwicklung eines mechanischen Ersatzmodells zur Beschreibung gesinterter Keramiken
Master Thesis, Ruhr-Universität Bochum (2015)

>> Theses 2016

S. Gao
3D discrete dislocation dynamics study on fundamental creep mechanisms in single crystal superalloys
PhD Thesis, Ruhr-Universität Bochum (2016)

P. S. Engels
A multi-phase-field simulation approach incorprating finite, eslasto-plastic deformations
PhD Thesis, Ruhr-Universität Bochum (2016)

H. R. Hajiyani
Mechanical and electrochemical properties of mixed transition metal oxides in cathode materials
PhD Thesis, Ruhr-Universität Bochum (2016)

R. Hameed
Micromechanical modeling of strength of tempered martensitic steels based on crystal plasticity
PhD Thesis, Ruhr-Universität Bochum (2016)

M. Boeff
Micromechanical modelling of fatigue crack initiation and growth
PhD Thesis, Ruhr-Universität Bochum (2016)

G. Du
Phase-field simulation of lath martensite in low-carbon steel
PhD Thesis, Ruhr-Universität Bochum (2016)

A. Monas
Phase-field simulation of morphology evolution during eutectic solidification
PhD Thesis, Ruhr-Universität Bochum (2016)

M. Kulosa
Modellierung der elastischen und thermischen Eigenschaften sowie des Schädigungsverhaltens poröser partikelbasierter Keramiken
PhD Thesis, Ruhr-Universität Bochum (2016)

J. Wang
Structural transformations in Fe-C alloys: Atomistic modeling of grain boundaries and segregation in α iron
PhD Thesis, Ruhr-Universität Bochum (2016)

S. Schreiber
Simulation of plastic deformation in α-FeC with analytic bond-order potentials
PhD Thesis, Ruhr-Universität Bochum (2016)

R. Sivanesapillai
Pore-scale study of non-Darcian fluid flow in porous media using smoothed-particle hydrodynamics
PhD Thesis, Ruhr-Universität Bochum (2016)

V. Bhogireddy
Liquid metal induced grain boundary embrittlement: A multi-scale study
PhD Thesis, Ruhr-Universität Bochum (2016)

A. K. Vatti
An ab initio study of muscovite mica and formation energy of ions in liquid water
PhD Thesis, Ruhr-Universität Bochum (2016)

S. Surendralal
Automated calculations for charged point defects in magnesium oxide and iron oxides
Master Thesis, Ruhr-Universität Bochum (2016)

V. Begum
Parallelization of Wolff single-cluster algorithm in 2D Ising model with MPI
Master Thesis, Ruhr-Universität Bochum (2016)

A. Asaadi
Molecular dynamics simulations of nano-indentation in lamellar γ-γ′ microstructures of TiAl
Master Thesis, Ruhr-Universität Bochum (2016)

P. L. Veluvali
Influence of interstitial defects on the structural and mechanical properties of lamellar TiAl alloys
Master Thesis, Ruhr-Universität Bochum (2016)

M. Dakshinamurthy
Micromechanical modeling of the effect of transformation induced plasticity on crack propagation in multiphase steels
Master Thesis, Ruhr-Universität Bochum (2016)

A. Puchakayala Appaiah Subramanyam
A first principles study of effects of manganese on hydrogen embrittlement of a carbon segregated E5 (310)[00]) grain boundary in α iron
Master Thesis, Ruhr-Universität Bochum (2016)

S. Abbas
Size effect in mechanical properties of multilayered material by accumulative roll bonding
Master Thesis, Ruhr-Universität Bochum (2016)

P. Camargos Macieira
Simulation of microstructure evolution during hot rolling of VDM alloy 718
Master Thesis, Ruhr-Universität Bochum (2016)

M. U. Bilal
Growth kinetics and coherency loss from θ′ to θ in Al-Cu alloy: A phase-field study
Master Thesis, Ruhr-Universität Bochum (2016)

H. Heyn
Molecular Dynamics Simulation of nanoindentation of cc and bcc systems: Influence of hydrogen on vacancies
Master Thesis, Ruhr-Universität Bochum (2016)

F. Kazemi
Effect of Boron additions during dendritic solidification on the microstructure properties and mechanical properties
Master Thesis, Ruhr-Universität Bochum (2016)

S. Papenkort
Simulation von Ermüdungsrisswachstum in polykristallinen Mikrostrukturen unter zyklischer Belastung / Simulation of fatigue crack growth in polycrystalline microstructures under cyclic loading conditions
Master Thesis, Ruhr-Universität Bochum (2016)

C. Steger
Optimierung des Lagenaufbaus für ein Monocoque in Sandwichbauweise
Master Thesis, Ruhr-Universität Bochum (2016)

T. Lyu
Microstructure and micromechanical modelling of Al-Cu dissimilar material connections
Master Thesis, Ruhr-Universität Bochum (2016)

M. F. Schröder
Lattice dynamics in hybrid-perovskites
Master Thesis, Ruhr-Universität Bochum (2016)

E. Turchenko
Automated data proceeding and its application to creep experiments
Master Thesis, Ruhr-Universtität Bochum (2016)

Talks and Posters

15. Talks and Posters

>> Invited talks 2015

02.01.2015
A. Hartmaier, K. Chockalingam, R. Hameed, P. Schwittek, R. Janisch, A. Ma
Atomistically informed continuum models for plasticity and fracture of tempered martensite
International Symposium of Plasticity 2015, Montego Bay, Jamaica

04.01.2015
I. Steinbach, E. Borukhovich, A. A. Gießmann, P. S. Engels
Phase-field model of solid state transformations with large distortion and plastic activity
International Symposium of Plasticity 2015, Montego Bay, Jamaica

05.01.2015
A. Ma, A. Hartmaier
The higher order nonlocal constitutive model and its application to multiphase materials
International Symposium of Plasticity 2015, Montego Bay, Jamaica

07.01.2015
J. Rogal
Structural phase transformations in solids: Atomistic insight on mechanisms and interface properties
International Conference on Computational Physics, Singapore

19.01.2015
S. G. Fries
Thermodynamic modeling as a link between basic and applied science
Indian Institute of Technology, Madras, India

26.02.2015
R. Janisch
Energies and mechanical properties of interfaces from ab-initio calculations and their use in mesoscale models
Thomas Young Centre, London, UK

06.03.2015
G. Madsen
Integrated computational materials discovery of new thermoelectric materials
APS March Meeting 2015, San Antonio, USA

16.03.2015
J. Rogal
Modelling solid-solid phase transformations: Atomistic insight on mechanisms and interface properties
DPG Spring Meeting 2015, Berlin, Germany

26.03.2015
M. Boeff
Implementation of a coupled plasticity-damage model into a spectral solver
3rd Meeting of the Jung-DGM Group Rhein-Ruhr, Dortmund, Germany

26.03.2015
I. Steinbach
Why solidification? Why phase-field?
Imperial College, London, UK

09.04.2015
R. Drautz
Bond-order potentials: From the electronic structure to transferable interatomic potentials
Linköping University, Sweden

20.04.2015
S. Bhattacharya, G. Madsen
Achieving optimum doping in p-type SnS thermoelectrics
Denmark Technical University, Lyngby, Denmark

21.04.2015
B. Wu, N. Vajragupta, J. Lian, Y. Duan, T. Lertsirarungsun, U. Hangen, S. Münstermann
FE simulation of nanoindentation tests with crystal plasticity finite element method and virtual experiment
Hysitron Nanobrücken Workshop and User Meeting 2015, Potsdam, Germany

02.06.2015
I. Steinbach
Why solidification? Why phase-field?
Universität Bremen, Bremen, Germany

05.06.2015
G. Madsen
Controlling the charge carrier concentration
SPP 1386 Nanostructured Thermoelectrics Symposium, Hamburg, Germany

08.06.2015
G. Madsen
High-throughput evaluation of thermoelectric powerfactors
CECAM Workshop Future Technologies in Automated Atomistic Simulations, Lausanne, Switzerland

10.06.2015
S. Bhattacharya
Material design strategies to search for effecient thermoelectrics
IMRA Europe Research Institute, Sophia Antipolis, France

22.06.2015
R. Janisch
Can we model the mechanical properties of grain boundaries based on a few material properties?
Workshop on Understanding Grain Boundary Migration: Theory Meets Experiment, Günzburg, Germany

23.06.2015
T. Hammerschmidt, J. Koßmann, R. Drautz
Topologically close-packed phases in Co-based superalloys
International Workshop on Advanced Co-based Superalloys, National Institute of Standards and Technology, Gaithersburg, USA

24.06.2015
M. Palumbo
A DFT-based consistent thermodynamic database for Co/Ni systems
International Workshop on Advanced Co-based Superalloys, National Institute of Standards and Technology, Gaithersburg, USA

25.06.2015
G. Madsen
Good vibrations: Thermal conductivity from Boltzmann transport theory
GHI-Sommerkolloquium Werkstoffcharakterisierung, Aachen, Germany

29.06.2015
I. Steinbach
PTM 2015: Pearlite revisited
Solid-Solid Phase Transformations in Inorganic Materials, Whistler, Canada

07.07.2015
J. V. Görler, O. Shchyglo, S. Brinckmann, L. Mujica, I. Lopez-Galilea, W. Theisen, I. Steinbach
Phase-field simulation of long-term aging in nickel-base superalloys
ESMC 2015, Universidad Carlos III, Madrid, Spain

15.07.2015
R. Drautz
From the electronic structure to transferable interatomic potentials
CECAM Workshop Next Generation Quantum Based Molecular Dy-Namics: Challenges and Perspectives, Bremen, Germany

16.07.2015
M. Palumbo
DFT-based thermodynamic modelling of Ni and Co-base superalloys
Departmental Lunch Colloquium of the Department of Materials Science and Engineering, Delft University of Technology, Delft, The Netherlands

16.07.2015
J. Koßmann, T. Hammerschmidt, R. Drautz
Comparing Co-based and Ni-based superalloys with density-functional theory
Departmental Lunch Colloquium of the Department of Materials Science and Engineering, Delft University of Technology, Delft, The Netherlands

27.07.2015
A. Ma, A. Hartmaier
Microstructure informed constitutive models and their applications
Ohio State University, Columbus, USA

20.08.2015
R. Drautz, I. Opahle, T. Chakraborty, J. Rogal
On the effect of Ni on the martensitic transformation temperatures in near equiatomic NiTi alloys
20+1 Symposium, Bochum, Germany

01.09.2015
J. Rogal
Capturing the kinetics of complex phase boundary migration: An adaptive kinetic Monte Carlo study
CECAM Workshop Chemical and Structural Transformations in Materials Under Mechanical Load, Lausanne, Switzerland

06.09.2015
G. Madsen
Evaluation of thermoelectric descriptors
PSI-k 2015, San Sebastian, Spain

09.09.2015
R. Drautz
Analytic bond-order potentials: From a simplified description of the electronic structure to structural stability in elements and compounds
PSI-k 2015, San Sebastian, Spain

18.09.2015
M. Staadt
Free energy Monte Carlo sampling with bond-order potentials
University of California, Berkeley, USA

22.09.2015
R. Drautz
Bond-order potentials: From the electronic structure to transferable interatomic potentials
Euromat 2015, Warsaw, Poland

06.10.2015
A. Hartmaier
Micromechanical modeling (I. heterogeneous materials, II. microstructure evolution)
French-German Summer School on Evolutionary Solid Bodies, Bollendorf, Germany

21.10.2015
S. Münstermann, G. Golisch, B. Wu
A hybrid damage mechanics model to predict the impact toughness of structural steel
Bao Steel Conference 2015, Shanghai, China

28.10.2015
R. Drautz
From the electronic structure to transferable interatomic potentials
ESTADSM 2015, Moscow, Russia

30.10.2015
A. Hartmaier
Atomistically informed continuum models for plasticity, damage and fracture of martensitic steels
International Symposium on Microstructure and Mechanical Properties of Advanced Metallic Materials, Erlangen, Germany

10.11.2015
I. Steinbach
Phase-field simulation of non-equilibrium processes at the mesoscopic scale
CECAM/Psi-k/HERALD Workshop SimGrow 2015, Marburg, Germany

11.11.2015
G. Madsen
Thermoelectric power factors by design
EPSRC Thermoelectric Network Meeting, Reading, UK

12.11.2015
G. Madsen
Computational techniques for the calculation of electronic transport coefficients
EPSRC Thermoelectric Network Meeting, Reading, UK

13.11.15
S. G. Fries, M. Palumbo
4000 and almost 100 years old materials, all new for DFT: Steels and Ni/Co-based super alloys
Imperial College, London, UK

30.11.2015
T. Hammerschmidt
Descriptors for the structural stability of sp-d valent compounds
CECAM Workshop Big Data of Materials Science, Lausanne, Switzerland

09.12.2015
T. Hammerschmidt
Robust crystal structure with structure maps
Friedrich-Schiller Universität, Jena, Germany

>> Invited talks 2016

04.02.2016
S. Bhattacharya
Material design strategies for thermoelectrics
INNI-CECAM Workshop, Tel Aviv, Israel

02.03.2016
A. Hartmaier
Atomistically informed crystal plasticity models
Schöntal Symposium Dislocation-based Plasticity, Schöntal, Germany

08.03.2016
T. Hammerschmidt
Robust crystal-structure prediction with structure maps
DPG Spring Meeting, Regensburg, Germany

12.04.2016
R. Darvishi Kamachali
Studying microstructure evolution using phase-field method
Bundesanstalt für Materialforschung und –prüfung, Berlin, Germany

27.04.2016
R. Janisch
Grain boundary properties from atomistic simulations and their use in mechanical modelling of materials
Physikalisches Kolloquium at the Institute of Physics, TU Chemnitz, Germany

28.04.2016
R. Janisch
Grain boundary properties from atomistic simulations and their use in mechanical modelling of materials
Fraunhofer IWS Seminar, Dresden, Germany

12.05.2016
A. Hartmaier
What does nanoscale testing and modeling teach us on macroscopic material behavior?
Colloquium of the Department of Materials, University of Oxford, UK

14.05.2016
I. Steinbach
Why solidification? Why phase-field?
CSSCR 2016: 4th International Symposium on Cutting Edge of Computer Simulation of Solidification, Casting and Refining, Xi'an, Republic of China

02.06.2016
M. Stratmann, O. Shchyglo, L. Zhang, I. Steinbach
Unifying the CALPHAD sublattice model and the phase-field model with finite interface dissipation
CALPHAD XLV, Awaji Island, Hyogo, Japan

14.06.2016
S. Münstermann, B. Wu, J. Lian
An extension of the modified Bai Wierzbicki model to non-proportional loading
IDDRG Conference 2016: Challenges in Forming High-Strength Sheets, Linz, Austria

22.06.2016
Z. Xu, F. Fang, Y. Xiao, T. Wang, A. Hartmaier
Molecular dynamics simulation of focused Ga ion beam induced nanoscale damage on silicon and its annealing recovery mechanism
EMN 2016: Energy Materials and Nanotechnology, Prague, Czech Republic

28.06.2016
A. Hartmaier
Atomistically informed continuum models for plasticity and fracture
8th International Conference on Materials Structure and Micromechanics of Fracture, Brno, Czech Republic

05.07.2016
E. Borukhovich, M. Boeff, A. Monas, M. Tegeler, S. Kim, C. Oh, I. Steinbach
Full-field simulation of solidification and forming of polycrystals
Numiform 2016, Troyes, France

07.07.2016
S. Bhattacharya
Material design challenges in predicting a novel thermoelectric
Forschungszentrum Jülich, Germany

18.07.2016
R. Drautz
Coarse graining of the electronic structure for atomistic modelling of high-temperature materials
Beyond Nickel-Based Superalloys II,Cambridge, UK

09.08.2016
J. Rogal
Rare event dynamics in materials science
Universidad Nacional Autonoma de Mexico, Mexico City, Mexico

25.08.2016
S. G. Fries
The thermodynamics of high temperature materials supported by DFT calculations
Special Seminar at the School of Computing, Science and Engineering, Salford, UK

01.09.2016
R. Janisch
Verformung an Grenzflächen in Al und TiAl: Was lernen wir aus atomistischen Simulationen?
DGM Regionalforum Rhein-Ruhr, Bonn, Germany

04.09.2016
S. Bhattacharya
Predicting a novel thermoelectric material: Material design challenges
26th Conference, Groningen, The Netherlands

09.09.2016
Z. Xu, F. Fang, A. Hartmaier
Ion beam nanofabrication and its applications in nano-optics and bio-sensing
Special Seminar at Cardiff University, Cardiff, UK

27.09.2016
A. Hartmaier, C. Begau, G. Sutmann
Free energy function of dislocation densities by large scale atomistic simulation
MSE 2016: Materials Science and Engineering Congress, Darmstadt, Germany

14.10.2016
R. Drautz
Intermediate models for bridging from high-throughput data to materials properties
8th International Conference on Multiscale Materials Modeling, Dijon, France

20.10.2016
A. Hartmaier
Atomistically informed continuum models for deformation and fracture of materials
MICOS 2016: International Conference on Microscale Morphology of Component Surfaces, TU Kaiserslautern, Germany

24.10.2016
S. G. Fries
Thermodynamic modeling using small data
Materials Science and Technology: Technical Meeting 2016, Salt Lake City, USA

27.10.2016
M. Mrovec
New insights into hydrogen trapping and diffusion in metallic microstructures obtained from atomistic simulations
Atomic scale modeling: What's in for steel?, Ghent, Belgium

01.12.2016
A. Hartmaier
Virtuelle und reale Härteprüfung: Wie gelingt die Verknüpfung von Experiment und Simulation?
Tagung Werkstoffprüfung 2016, Neu-Ulm, Germany

15.12.2016
D. G. Sangiovanni
Mass transport and plastic deformation in refractory nitrides: Density functional theory and ab initio molecular dynamics
Pacific Rim Symposium of Surfaces, Coatings and Interfaces, Big Island Hawaii, USA

>> Talks and posters 2015

19.01.2015
G. Díaz Leines, R. Drautz, J. Rogal
Nucleation during solidification in Ni: Atomistic insight from transition path sampling simulations
Computational Materials Science on Complex Energy Landscapes, Kirchdorf, Austria

20.01.2015
A. C. Ladines, T. Hammerschmidt, R. Drautz
Bond-order potential for Fe-Nb
Computational Materials Science on Complex Energy Landscapes, Kirchdorf, Austria

22.01.2015
R. Stern, S. Bhattacharya, G. Madsen
Carrier concentration controlling point defects in NiTiSn half-Heusler structures
Computational Materials Science on Complex Energy Landscapes, Kirchdorf, Austria

22.01.2015
S. Bhattacharya, G. Madsen
High-throughput materials design strategy for thermoelectrics
Computational Materials Science on Complex Energy Landscapes, Kirchdorf, Austria

22.02.2015
A. Katre, G. Madsen
Simplified models for thermal transport in nanostructured materials
SPP 1386 Nanostructured Thermoelectrics Status Meeting, Bad Aussee, Austria

24.02.2015
I. Steinbach
Strong coupling of thermochemical and thermomechanical states in applied science
Spring Meeting of the DGM Workgroup Mechanics of Microstructure, Kassel, Germany

02.03.2015
S. Bhattacharya, G. Madsen
High-throughput materials design strategy for thermoelectrics
APS March Meeting 2015, San Antonio, USA

16.03.2015
J. Albina, A. Marusczyk, T. Hammerschmidt, R. Drautz
Modeling the structural stability during delithiation in Li-Mn-Ni oxides from first-principles
DPG Spring Meeting 2015, Berlin, Germany

16.03.2015
I. Opahle, J. Frenzel, A. Wieczorek, B. Maaß, G. Eggeler, R. Drautz
Density functional investigations on the effect of Ni excess in binary Ni-Ti shape memory alloys
DPG Spring Meeting 2015, Berlin, Germany

16.03.2015
A. M. Tahir, R. Janisch, A. Hartmaier
Hydrogen embrittlement of a carbon segregated symmetrical tilt grain boundary in α-Fe
DPG Spring Meeting 2015, Berlin, Germany

16.03.2015
S. Schuwalow, J. Rogal, R. Drautz
Diffusion of solutes in Ni-based superalloys: Role of vacancies and the treatment of the non-dilute limit
DPG Spring Meeting 2015, Berlin, Germany

17.03.2015
R. Stern, G. Madsen
First principles calculations of point defects to optimize the thermoelectric efficiency of half-Heusler compounds
DPG Spring Meeting 2015, Berlin, Germany

17.03.2015
A. Bialon, T. Hammerschmidt, R. Drautz
Structure map for crystal-structure prediction of sp-d valent compounds
DPG Spring Meeting 2015, Berlin, Germany

17.03.2015
T. Schablitzki, J. Rogal, R. Drautz
Thermal desorption spectra from 3D materials
DPG Spring Meeting 2015, Berlin, Germany

17.03.2015
S. Bhattacharya, S. Jacobs, N. S. Gunda, R. Stern, R. Chmielowski, G. Dennler, G. Madsen
Achieving optimum doping in p-type SnS thermoelectrics
DPG Spring Meeting 2015, Berlin, Germany

18.03.2015
R. Schiedung, I. Steinbach, U. Köhler
Annealing of copper nanoparticles on substrate by surface diffusion
DPG Spring Meeting 2015, Berlin, Germany

18.03.2015
T. Chakraborty, J. Rogal, R. Drautz
First principles study of competing phases in binary Ti-Ta alloys
DPG Spring Meeting 2015, Berlin, Germany
18.03.2015

S. Sampath, R. Janisch
Influence of alloying elements on the fracture strength of iron
DPG Spring Meeting 2015, Berlin, Germany

18.03.2015
T. Schablitzki, J. Rogal, R. Drautz
Characterisation of transformations at disordered FeCr bcc-σ interfaces
DPG Spring Meeting 2015, Berlin, Germany

18.03.2015
G. Díaz Leines, R. Drautz, J. Rogal
Exploring nucleation mechanisms in nickel: Novel insight from transition path sampling simulations
DPG Spring Meeting 2015, Berlin, Germany

19.03.2015
J. Wang, G. Madsen, R. Drautz
First-principles and tight-binding studies of symmetrical tilt grain boundaries in bcc-Fe
DPG Spring Meeting 2015, Berlin, Germany

19.03.2015
M. Kanani, R. Janisch, A. Hartmaier
Shearing behaviour of interfaces: Linking intrinsic properties with deformation mechanisms
DPG Spring Meeting 2015, Berlin, Germany

20.03.2015
I. Opahle, G. Madsen, R. Drautz
Density functional and tight-binding analysis of the energy balance between $L1_0$ and $L2_1$ structures in Ni-Mn-*X*(*X*=Ga, Sn, In) Heusler alloys
DPG Spring Meeting 2015, Berlin, Germany
25.03.2015

A. Ma, I. Lopez-Galilea, W. Theisen, A. Hartmaier
CPFEM modeling of porosity reduction in an as-cast Ni-base single crystal superalloy under HIP
Gordon Research Conference Physical Metallurgy 2015, Maine, USA

25.03.2015
M. Tegeler, A. Monas, G. Sutmann
Massively parallel multiphase field simulations
4th International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering, Dubrovnik, Croatia

25.03.2015
C. Teijeiro Barjas, T. Hammerschmidt, R. Drautz, G. Sutmann
Parallel bond order potentials for materials science simulations
4th International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering (PARENG 2015), Dubrovnik, Croatia

30.03.2015
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Precipitation processes in aluminium alloys
SiMiDe SpringSchool 2015 on Phase Transformations, Hammin-keln, Germany

27.04.2015
M. Staadt, J. Rogal, T. Hickel, R. Drautz, J. Neugebauer
Sampling of iron free energy using embedded atom and bond-order potentials
IMPRS-SurMat Workshop, Düsseldorf, Germany

04.05.15
F. Varnik
Correlation of motion and diffusion in sheared athermal suspensions of deformable particles
International Workshop on Dynamics in Viscous Liquids, Montpellier, France

05.05.15
M. R. Hassani, D. Raabe, F. Varnik
Sensitivity of the correlation plastic rearrangements to the microscopic dynamics in sheared disordered solids
International Workshop on Dynamics in Viscous Liquids, Montpellier, France

05.05.15
F. Varnik, D. Raabe
Non-locality of effective temperature in a shear driven model glass
International Workshop on Dynamics in Viscous Liquids, Montpellier, France

06.05.2015
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field simulation of precipitation processes in aluminium alloys
10th Seminar of the SiMiDe Graduate School, Bochum, Germany

12.05.2015
S. Gao, M. Fivel, A. Hartmaier
Influence of misfit stresses on dislocation glide in single crystal superalloys: A three-dimensional discrete dislocation dynamics study
12th International Conference on the Mechanical Behavior of Materials, Karlsruhe, Germany

12.05.2015
A. Ma, S. Gao, I. Lopez-Galilea, S. Huth, W. Theisen, A. Hartmaier
Crystal plasticity modeling of porosity reduction in an as-cast Ni-base single crystal superalloy during hot isostatic pressing
12th International Conference on the Mechanical Behavior of Materials, Karlsruhe, Germany

25.05.2015
I. Steinbach, E. Borukhovich, P. S. Engels
Phase-field model of solid state transformations with large distortion and plastic activity
2015 Bilateral Symposium of the Sino-German Cooperation Group Microstructure in Al Alloys & 1st Sino-German Symposium on Phase-Field Method and its Applications, Changsha, China

26.05.2015
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field simulation of aluminium precipitation hardening processes
2015 Bilateral Symposium of the Sino-German Cooperation Group Microstructure in Al Alloys & 1st Sino-German Symposium on Phase-Field Method and its Applications, Changsha, China

26.05.2015
M. Stratmann, O. Shchyglo, I. Steinbach
Phase-field simulation of precipitation in Cr and Mn alloyed martensitic steels
2015 Bilateral Symposium of the Sino-German Cooperation Group Microstructure in Al Alloys & 1st Sino-German Symposium on Phase-Field Method and its Applications, Changsha, China

27.05.2015
I. Roslyakova, H. Dette, I. Steinbach
Design of experiments for segmented heat capacity model
2015 Bilateral Symposium of the Sino-German Cooperation Group Microstructure in Al Alloys & 1st Sino-German Symposium on Phase-Field Method and its Applications, Changsha, China

28.05.2015
M. Kulosa, M. Neumann, M. Boeff, G. Gaiselmann, V. Schmidt, A. Hartmaier
Characterization of porous ceramics derived from a combination of stochastic and mechanical modeling
4th International Conference on Material Modeling, Berkeley, USA

07.06.2015
A. Katre, G. Madsen
Modelling thermal transport in nanostructured materials
Culminating Workshop of the IPAM Long Program Broad Perspectives and New Directions in Financial Mathematics, Los Angeles, USA

10.06.2015
R. Stern, G. Madsen
Optimized thermoelectric performance of half-Heusler materials by self- and isovalent doping
Materials for a Sustainable Energy Future Reunion Conference I, Lake Arrowhead, USA

16.06.2015
G. Díaz Leines, R. Drautz, J. Rogal
Nucleation during solidification in Ni: Atomistic insight from transition path sampling simulations
ICAMS Advanced Discussions 2015, Bochum, Germany

16.06.2015
C. Begau
Free energy function of dislocation densities in large scale atomistic simulations
ICAMS Advanced Discussions 2015, Bochum, Germany

16.06.2015
O. Shchyglo
Stress-strain sensitive Gibbs energy of alloys
ICAMS Advanced Discussions 2015, Bochum, Germany

16.06.2015
S. G. Fries
Thermodynamic descriptions including elastic properties for solid phases
ICAMS Advanced Discussions 2015, Bochum, Germany

24.06.2015
A. Monas, O. Shchyglo, D. Höche, I. Steinbach
Dual-scale phase-field simulation of Mg-Al alloy solidification
MCWASP XIV 2015, Awaji Island, Japan

30.06.2015
B. Sundman, U. R. Kattner, M. Palumbo, S. G. Fries
Advances in the development of OpenCalphad software and databases
PTM 2015: Solid Solid Phase Transformations in Inorganic Materials, Whistler, Canada

30.06.2015
O. Shchyglo, M. Mikolaychuk, I. Steinbach
Stress-strain: Sensitive Gibbs energy formulation of alloys
PTM 2015: Solid Solid Phase Transformations in Inorganic Materials, Whistler, Canada

16.07.2015
A. N. Harjunmaa, J. Rogal, R. Drautz, J. Duncan, R. Terrell, G. Henkelman
Capturing the kinetics of complex phase boundary migration: An adaptive kinetic Monte Carlo study
CECAM Workshop Next Generation Quantum Based Molecular Dynamics: Challenges and Perspectives, Bremen, Germany

27.07.2015
I. Steinbach, C. Schwarze, R. Darvishi Kamachali
Phase field study of Zener drag and pinning of cylindrical particles in nano-crystalline materials
5th Sino-German Symposium, Changchun, China

06.09.2015
A. Katre, G. Madsen
Tight binding model for thermal properties of Si nanostructures
PSI-k 2015, San Sebastian, Spain

07.09.2015
T. Hammerschmidt, A. Bialon, R. Drautz
Robust crystal-structure prediction with structure maps
PSI-k 2015, San Sebastian, Spain

07.09.2015
T. Chakraborty, J. Rogal, R. Drautz
Martensitic transformation in Ti-Ta: A first principles study
PSI-k 2015, San Sebastian, Spain

07.09.2015
S. Bhattacharya, G. Madsen
High-throughput search for efficient thermoelectrics
PSI-k 2015, San Sebastian, Spain

08.09.2015
R. Stern, S. Bhattacharya, G. Madsen
Optimized thermoelectric performance of half-Heusler materials by self- and isovalent doping
PSI-k 2015, San Sebastian, Spain

22.09.2015
H. Ganesan, C. Begau, G. Sutmann, A. Hartmaier
Atomistic modeling of carbon segregation and its influence on dislocation mobility in ferritic iron
EUROMAT 2015, Warsaw, Poland

23.09.2015
R. Darvishi Kamachali, S. Kim, I. Steinbach
Texture evolution in deformed AZ31 magnesium sheets: Experiments and phase-field study
Euromat 2015, Warsaw, Poland

23.09.2015
O. Shchyglo, E. Borukhovich, A. A. Gießmann, P. S. Engels, I. Steinbach
Phase-field model of solid state transformations with large deformation and plastic activity
Euromat 2015, Warsaw, Poland

23.09.2015
M. K. Rajendran, O. Shchyglo, I. Steinbach
Phase-field study of the effect of creep on the rafts formation in Ni-base superalloys
Euromat 2015, Warsaw, Poland

24.09.2015
A. B. Subhedar, F. Varnik, I. Steinbach
Modelling the flow in diffuse interface methods of solidification
Euromat 2015, Warsaw, Poland

28.09.2015
T. Hammerschmidt, J. Koßmann, A. C. Ladines, R. Drautz
Modelling topologically close-packed phases in superalloys and steels
Intermetallics 2015, Bad Staffelstein, Germany

02.10.2015
E. Borukhovich, I. Steinbach
Large deformation and its effect on the microstructure evolution
25th International Workshop on Computational Micromechanics, Bochum, Germany

02.10.2015
L. Moj, T. Ricken, I. Steinbach
A continuum-mechanical bi-phasic, two-scale model for thermal driven phase transition during solidification
25th International Workshop on Computational Micromechanics, Bochum, Germany

02.10.2015
X. Pang, A. M. Tahir, R. Janisch, A. Hartmaier
Interplanar potential for tension-shear coupling at grain boundaries from ab initio calculations
25th International Workshop on Computational Micromechanics, Bochum, Germany

05.10.2015
C. Begau, G. Sutmann, A. Hartmaier
Free energy function of dislocation densities by large scale atomistic simulations
Nanomechanical Testing in Materials Research and Development V, Albufeira, Portugal

08.10.2015
R. Schiedung
Surface diffusion of copper nanoparticles on substrate
Talk at Central-South University, Changsha, China

08.10.2015
R. Darvishi Kamachali
Precipitation and phase-field modeling
Talk at Korean Institute of Materials Science, Changwon, South Korea

09.10.2015
I. Roslyakova
Contribution to the third generation CALPHAD databases: Segmented model for pure Al, Cr, Ge, Ir, Mo, Nb, Re, W, Fe, Ni and statistical evaluation of the existing physically-based models
Central-South University, Changsha, China

12.10.2015
J. Jenke, A. C. Ladines, T. Hammerschmidt, D. G. Pettifor CBE FRS, R. Drautz
Tight-binding model for sp- and sd-valent dimers
Development of Next Generation Accurate Approximate DFT/B Methods, Bremen, Germany

13.10.2015
A. Monas, O. Shchyglo, C. Yim, I. Steinbach
Phase-field simulation of Mg-Al alloy solidification
10th International Conference on Magnesium Alloys and Their Applications, Jeju, South Korea

19.11.2015
H. Ganesan, C. Begau, G. Sutmann, A. Hartmaier
Atomistic modeling of carbon segregation and its influence on dislocation mobility in ferritic iron
RUB Research Day 2015, Bochum, Germany

30.11.2015
J. Duncan, A. N. Harjunmaa, R. Terrell, R. Drautz, G. Henkelmann, J. Rogal
Capturing the kinetics of complex phase boundary migration: An adaptive kinetic Monte Carlo study
MRS Fall Meeting 2015, Boston, USA

01.12.2015
G. Díaz Leines, R. Drautz, J. Rogal
Nucleation during solidification in Ni: Novel atomistic insight from transition path sampling simulations
MRS Fall Meeting 2015, Boston, USA

>> Talks and posters 2016

07.03.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Sampling free energies of different phases in Fe including atomic and magnetic degrees of freedom
DPG Spring Meeting, Regensburg, Germany

08.03.2016
J. Jenke, A. C. Ladines, T. Hammerschmidt, D. G. Pettifor CBE FRS, R. Drautz
Tight-binding parameterizations across the periodic table
DPG Spring Meeting, Regensburg, Germany

08.03.2016
N. Wang, T. Hammerschmidt, R. Drautz
Wurtzite to rocksalt phase transitions in binary compounds
DPG Spring Meeting, Regensburg, Germany

09.03.2016
J. Wang, G. Madsen, R. Drautz
First-principles study of carbon segregation in bcc iron symmetrical tilt grain boundaries
DPG Spring Meeting, Regensburg, Germany
10.03.2016

G. Díaz Leines, R. Drautz, J. Rogal
Atomistic insight into the structure and shape of growing nuclei during solidification in Ni
DPG Spring Meeting, Regensburg, Germany

31.03.2016
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field simulation of mechano-chemical coupling during precipitation in aluminum alloys
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, Republic of Korea

01.04.2016
R. Darvishi Kamachali
Phase-field and mean field study of grain growth and recrystallization
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, Republic of Korea

01.04.2016
R. Darvishi Kamachali
OpenPhase - the open source phase field simulation library
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, Rupublic of Korea

03.04.2016
B. Dongre
Predictive all-scale lattice thermal conductivity
WE-Heraeus-Seminar on Electrons and Phonons: Interfaces and Interactions, Bad Honnef, Germany

05.04.2016
R. Stern, G. Madsen
Thermal transport properties of FeSi alloys
WE-Heraeus-Seminar on Electrons and Phonons: Interfaces and Interactions, Bad Honnef, Germany

05.04.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Metropolis Monte Carlo sampling in Fe including atomic and magnetic degrees of freedom
SurMat Seminar, Altenkirchen, Germany

02.05.2016
S. Bhattacharya, G. Madsen
Designing efficient p-type half-Heusler thermoelectrics
MRS Spring Meeting, Lille, France

02.05.2016
J. Duncan, A. N. Harjunmaa, R. Terrel, R. Drautz, G. Henkelman, J. Rogal
Capturing the kinetics of complex phase boundary migration: An adaptive kinetic Monte Carlo study
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Sampling atomic and magnetic degrees of freedom in Fe using bond-order potentials
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
T. Hammerschmidt
Robust crystal-structure prediction with structure maps
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
R. Janisch
Constitutive relationships for interfaces from atomistic simulations
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
M. Boeff
Investigation of the influence of microstructure on fatigue crack initiation and growth using crystal plasticity simulations
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
J. Wang
First-principles study of carbon segregation in bcc-Fe symmetrical tilt grain boundaries
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
H. Ganesan
Carbon segregation in ferritic iron using a coupled Molecular Dynamics and Monte Carlo approach
ICAMS Advanced Discussions 2016, Bochum, Germany

02.05.2016
T. Chakraborty
Prediction of the martensite start temperature for the design of high-temperature shape memory alloys
ICAMS Advanced Discussions 2016, Bochum, Germany

03.05.2016
J. Albina
Modeling the structural stability during delithiation in battery materials from first-principles
ICAMS Advanced Discussions 2016, Bochum, Germany

03.05.2016
T. Schablitzki
Temperature programmed desorption spectra for 3D materials
ICAMS Advanced Discussions 2016, Bochum, Germany

03.05.2016
I. Roslyakova
Automated data processing and its application to creep experiments
ICAMS Advanced Discussions 2016, Bochum, Germany

03.05.2016
A. Monas
Mg-base alloy modelling: From solidification to mechanical testing
ICAMS Advanced Discussions 2016, Bochum, Germany

03.05.2016
M. Stratmann
Unifying the CALPHAD sublattice model and the phase-field model with finite interface dissipation
ICAMS Advanced Discussions 2016, Bochum, Germany

03.05.2016
R. Darvishi Kamachali
Microstructure design in precipitation-hardened alloys
ICAMS Advanced Discussions 2016, Bochum, Germany

05.05.2016
M. Ghasemi, S. G. Fries, M. Stankovski, J. Johansson
First-principles study and thermodynamic modelling of foreign impurities and native defects in GaAs
MRS Spring Meeting, Lille, France

16.05.2016
S. G. Fries, A. A. Breidi
Mechanical properties of Ni-based solid solutions calculated from first-principles
Seminar at NanoLund Center for Nanoscience, Lund University, Sweden

30.05.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Simultaneous sampling of atomic and magnetic degrees of freedom in iron using bond-order potentials
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
G. Díaz Leines, R. Drautz, J. Rogal
Atomistic simulations of nucleation during solidification in nickel
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
T. Chakraborty, J. Rogal, R. Drautz
Insight in Ti-Ta high-temperature shape memory alloys from first-principles
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
I. Roslyakova, S. Zomorodpoosh, H. Dette, I. Steinbach
The third generation CALPHAD databases: Segmented model for pure Al, Cr, Ge, Ir, Mo, Nb, Re, W, Fe, Ni and Ta
Calphad XLV, Awaji Island, Hyogo, Japan

30.05.2016
N. Wang, T. Hammerschmidt, J. Rogal, R. Drautz
Spin dynamics with analytic bond-order potentials
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
R. Darvishi Kamachali
Phase field simulation of microstructure evolution: Grain growth, ripening and related issues
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
J. Jenke
Tight-binding parameterizations across the periodic table
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
T. Schablitzki
Characterisation of transformation paths at disordered FeCr bcc-interfaces
Materials Chain International Conference 2016, Bochum, Germany

30.05.2016
F. Varnik
Scale bridging modelling of complex fluids: From nano-scale flow to suspension rheology
Materials Chain International Conference 2016, Bochum, Germany

31.05.2016
R. Janisch, X. Pang, M. Kanani, A. Hartmaier
Constitutive relationships for grain boundaries from atomistic simulations for multiscale mechanical modelling of metallic microstructures
Materials Chain International Conference 2016, Bochum, Germany

31.05.2016
J. Duncan, A. N. Harjunmaa, R. Terrel, R. Drautz, G. Henkelman, J. Rogal
Capturing the kinetics of complex phase boundary migration: An adaptive kinetic Monte Carlo study
Materials Chain International Conference 2016, Bochum, Germany

31.05.2016
I. Roslyakova
The third generation CALPHAD databases: Mo-Nb-Ta phase diagram with the segmented model
Calphad XLV, Awaji Island, Hyogo, Japan

31.05.2016
T. Hickel
Ab initio predicted phase stabilities of complex materials at finite temperatures
Materials Chain International Conference 2016, Bochum, Germany

31.05.2016
A. Hartmaier
Advances in scalebridging modeling of deformation and fracture in martensitic steels
Materials Chain International Conference 2016, Bochum, Germany

31.05.2016
G. Eggeler
Characterization and thermodynamic/kinetic analysis of nano-particles in microstructures of single crystal superalloys
Materials Chain International Conference 2016, Bochum, Germany

07.06.2016
R. Stern, G. Madsen
Thermal transport properties of FeSi alloys
IPAM Workshop on Materials for a Sustainable Energy Future, Lake Arrowhead, USA

08.06.2016
Z. Xu, F. Fang, A. Hartmaier
Diamond cutting tool's nanofabrication with focused ion beam
1st International Conference on Helium Ion Microscopy and Emerging Focused Ion Beam Technologies, Luxembourg

20.06.2016
S. Münstermann, M. Sharaf
A numerical approach to quantify the microstructure effect on the endurance fatigue strength of structural steel
21st European Conference on Fracture, Catania, Italy

20.06.2016
M. R. Hassani, D. Raabe, F. Varnik
Plasticity in amorphous solids: Local heterogeneity and localization of plastic deformations
Workshop on Hybrid Simulation Methods in Fluid Dynamics: Models, Software and Application, Garching, Germany

26.06.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Sampling atomic and magnetic degrees of freedom in Fe using bond-order potentials
Computational Materials Science Workshop, Domburg, The Netherlands

27.06.2016
J. Jenke, A. C. Ladines, T. Hammerschmidt, D. G. Pettifor CBE FRS, R. Drautz
Tight-binding parameterizations across the periodic table
Computational Materials Science Workshop, Domburg, The Netherlands

27.06.2016
G. Díaz Leines, J. Rogal
Comparison of minimum-action and steepest-descent paths in gradient systems
Computational Materials Science Workshop, Domburg, The Netherlands

27.06.2016
T. Chakraborty, J. Rogal, R. Drautz
Ab initio calculations for the design of novel Ti-Ta high-temperature shape memory alloys
Computational Materials Science Workshop, Domburg, The Netherlands

27.06.2016
N. Wang, T. Hammerschmidt, J. Rogal, R. Drautz
Spin dynamics with magnetic bond-order potentials
Computational Materials Science Workshop, Domburg, The Netherlands

29.06.2016
T. Wang
Phonon scattering induced by line defects in silicon viewed from Atomic-Green's-Function approach
NVM Workshop, Dublin, Ireland

18.07.2016
S. G. Fries, C. Zenk, N. J. Dupin, A. Markström, S. Neumeier, M. Göken
Evaluation of Co-based thermodynamic databases with respect to own and literature experimental data
Beyond Nickel-Based Superalloys Conference II, Cambridge, UK

26.07.2016
I. Roslyakova
Comparison of analytical solutions for the Debye model of heat capacity
Sino-German Symposium on Microstructure in Al Alloys, Bochum, Germany

05.09.2016
G. Díaz Leines, R. Drautz, J. Rogal
Nucleation during solidification in Ni: Novel atomistic insight from transition path sampling simulations
Nucleation: Past and Future Challenges for Experiment, Theory and Simulation, Buckinghamshire, UK

12.09.2016
Z. Xu, F. Fang, A. Hartmaier
Ion beam nanofabrication and its applications in bio-sensing & Si/SiC brittle materials' nanocutting under SEM
Seminar at Centre for Precision Manufacturing at the University of Strathclyde, Glasgow, UK

12.09.2016
T. Hammerschmidt, J. Koßmann, C. Zenk, S. Neumeier, M. Göken, I. Lopez-Galilea, L. Mujica, S. Huth, A. Kostka, W. Theisen, R. Drautz
The role of local chemical composition for TCP phase precipitation in Ni-base and Co-base superalloys
Superalloys 2016, Seven Springs, USA

14.09.2016
A. Hartmaier, P. Schwittek
Micromechanical modeling of hydrogen embrittlement in martensitic steel
International Hydrogen Conference 2016, Grand Teton National Park, USA

17.09.2016
R. Drautz
From electrons to materials
Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

26.09.2016
M. R. Hassani, D. Raabe, F. Varnik
From glass to supercooled liquid: Long-range correlation of shear strain persists
3rd International Workshop on Nonlinear Response in Complex Matter, Primošten, Croatia

26.09.2016
M. R. Hassani, D. Raabe, F. Varnik
From glass to supercooled liquid: Long-range correlation of shear strain persists
3rd International Workshop on Nonlinear Response in Complex Matter, Primošten, Croatia

27.09.2016
F. Varnik
The role of stress and structure fluctuations for plastic response
3rd International Workshop on Nonlinear Response in Complex Matter, Primošten, Croatia

27.09.2016
R. Janisch, M. Kanani, A. Hartmaier
Shear mechanisms at interfaces in lamellar TiAl alloys from atomistic simulations
MSE 2016: Materials Science and Engineering Congress, Darmstadt, Germany

28.09.2016
R. Janisch, A. Asaadi, A. Izardar, A. Hartmaier
Molecular dynamics simulations of nano-indentation in lamellar microstructures of TiAl
MSE 2016: Materials Science and Engineering Congress, Darmstadt, Germany

28.09.2016
E. Mahmoudinezhad Zirdehi, F. Varnik
Chemo-mechanical coupling in shape memory polymers: Theory versus experiment
MSE 2016: Materials Science and Engineering Congress, Darmstadt, Germany

28.09.2016
R. Darvishi Kamachali, C. Schwarze, I. Steinbach
Ripening and rearrangements of precipitates under mechano-chemical coupling
MSE 2016: Materials Science and Engineering Congress, Darmstadt, Germany

29.09.2016
A. Hartmaier, P. Schwittek
Micromechanical modeling of hydrogen embrittlement in martensitic steel
MSE 2016: Materials Science and Engineering Congress, Darmstadt, Germany

03.10.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Simultaneous sampling of atomic and magnetic degrees of freedom in iron using bond-order potentials
ADIS 2016, Tegernsee, Germany

03.10.2016
A. Puchakayala Appaiah Subramanyam, R. Janisch, A. Hartmaier
Effects of manganese on the hydrogen embrittlement of a Carbon segregated grain boundary in α-Fe
ADIS 2016, Tegernsee, Germany

04.10.2016
N. Wang, T. Hammerschmidt, J. Rogal, R. Drautz
Spin dynamics with magnetic bond-order potentials
ADIS 2016, Tegernsee, Germany

05.10.2016
M. Staadt, N. Wang, T. Hammerschmidt, J. Rogal, R. Drautz
From density functional theory to magnetic potentials and phase transformation kinetics
ADIS 2016, Tegernsee, Germany

09.10.2016
M. R. Hassani, F. Varnik
Shear banding in amorphous solids: The role of heterogeneity in structure and force distribution
8th International Conference on Multiscale Materials Modeling, Dijon, France

10.10.2016
G. Díaz Leines, J. Rogal
Comparison of minimum-action and steepest-descent paths in gradient systems
8th International Conference on Multiscale Materials Modeling, Dijon, France

11.10.2016
R. Darvishi Kamachali
Growth and ripening under mechanochemical coupling
8th International Conference on Multiscale Materials Modeling, Dijon, France

11.10.2016
T. Chakraborty, J. Rogal, R. Drautz
The martensitic transformation in Ti-Ta high-temperature shape memory alloy: Insight from first-principles calculations
8th International Conference on Multiscale Materials Modeling, Dijon, France

13.10.2016
T. Hammerschmidt, A. Bialon, R. Drautz
Three-parameter crystal-structure prediction for sp-d valent compounds
8th International Conference on Multiscale Materials Modeling, Dijon, France

13.10.2016
G. Díaz Leines, R. Drautz, J. Rogal
Transition path sampling simulations of nucleation during solidification in nickel
8th International Conference on Multiscale Materials Modeling, Dijon, France

13.10.2016
T. Wang
Phonon scattering caused by extended defects in silicon revealed from Atomic-Green's-Function approach
8th International Conference on Multiscale Materials Modeling, Dijon, France

25.10.2016
M. Staadt, J. Rogal, T. Hickel, T. Hammerschmidt, J. Neugebauer, R. Drautz
Simultaneous sampling of atomic and magnetic degrees of freedom in iron using bond-order potentials
Materials Day, Bochum, Germany

28.11.2016
T. Chakraborty, J. Rogal, R. Drautz
Ab initio calculations for the design of novel Ti-Ta high-temperature shape memory alloys
MRS Fall Meeting, Boston, USA

28.11.2016
T. Chakraborty, J. Rogal, R. Drautz
Ab initio investigation of Ti-Ta high-temperature shape memory alloys
MSE 2016, Hanover, Germany

Seminars and other Lectures

16. Seminars and other Lectures

>> Organisation and contribution to organisation of workshops and events 2015

23.06.2015 - 24.06.2015
International workshop on advanced Co-based superalloys
National Institute of Standards and Technology
Gaithersburg
Maryland, USA

16.06.2015
ICAMS Advanced Discussions: From Atoms to Continuum
Ruhr-Universität Bochum
Bochum
Germany

01.10.2015-02.10.2015
25th International Workshop on Computational Micromechanics of Materials
Ruhr-Universität Bochum
Bochum
Germany

>> Organisation and contribution to organisation of workshops and events 2016

31.03.2016 - 01.04.2016
Symposium on Simulation of Phase Transformation and Microstructure Evolution
Korea Institute of Materials Science
Changwon
Republic of Korea

02.05.2016 - 03.05.2016
ICAMS Advanced Discussions: Materials Design
Ruhr-Universität Bochum
Bochum
Germany

30.05.2016 - 01.06.2016
Materials Chain International Conference 2016
Ruhr-Universität Bochum
Bochum
Germany

03.10.2016 - 07.10.2016
ADIS 2016: Mechanical Properties
Schloss Ringberg
Kreuth
Germany

25.10.2016
Materials Day 2016
Ruhr-Universität Bochum
Bochum
Germany

08.11.2016
Trend-Workshop Skalenüberbrückende Simulation: Werkstoff, Prozess, Bauteil
Ruhr-Universität Bochum
Bochum
Germany

>> ICAMS IfM Seminars 2015

08.01.2015
Calculations of high-temperature properties of ceramic materials
M. Finnis
Imperial College, London, UK

15.01.2015
Shape memory thin films for medical and elastocaloric applications
E. Quandt
Christian-Albrechts-Universität zu Kiel, Germany

29.01.2015
Real dislocation dynamics
A. Sutton
Imperial College, London, UK

17.04.2015
Discovering materials for solar energy conversion
B. A. Parkinson
University of Wyoming, Laramie, USA

07.05.2015
Diffusion in high entropy alloys
S. V. Divinski
Westfälische Wilhelms-Universität Münster, Germany

18.06.2015
Cyclic contact deformation of metallic materials investigated by instrumented indentation
R. Schwaiger
Karlsruher Institut für Technologie, Germany

25.06.2015
New light shed on the dislocation-grain-boundary interaction
C. Kirchlechner
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

02.07.2015
Multiscale modelling of materials chemomechanics: From catastrophic brittle fracture to stress corrosion cracking
J. Kermode
University of Warwick, Coventry, UK

09.07.2015
FEM simulation in materials engineering – case studies in the field of heat treatment and life time prediction
C. Broeckmann
RWTH, Aachen, Germany

22.10.2015
Speeding up materials discovery through high-throughput ab initio computing
G. Hautier
Université Catholique, Louvain, Belgium

05.11.2015
Dislocation pattern formation and the similitude principle in a continuum theory of dislocation dynamics
S. Sandfeld
Friedrich-Alexander-Universität Erlangen-Nürnberg, Fürth, Germany

12.11.2015
Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy
B. Grabowski
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

19.11.2015
Very high cycle fatigue of engineering alloys
U. Krupp
University of Applied Sciences, Osnabrück, Germany

>> ICAMS IfM Seminars 2016

14.01.2016
Thermodynamics and precipitation in aluminum alloys: Presentation of the modeling tools used at Constellium
C. Sigli
Constellium C-TEC Grenoble, Grenoble, France

28.01.2016
Designing electronic phases at oxide interfaces for electronic, spintronic and energy applications
R. Pentcheva
Universität Duisburg-Essen, Duisburg, Germany

04.02.2016
Nanoimprinting of ultrafine-grained and nanocrystalline metals - How is plastic flow commencing in small-scaled cavities?
K. Durst
Technische Universität Darmstadt, Germany

21.04.2016
Solid surfaces - impact on mechanics and mechano-chemical coupling in small scale systems
J. Weissmüller
Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Haburg, Hamburg, Germany

19.05.2016
On the role of planar faults during creep of single crystal superalloys with γ/γ' microstructures
M. Titus
Max-Planck-Institut für Eisenforschung Düsseldorf, Germany

23.06.2016
On the mechanical behaviour of nonwovens
A. Ridruejo
Universidad Politécnica de Madrid, Spain

30.06.2016
Leicht und hochfest direkt aus der Schmelze: Gießwalzen am LWK
M. Schaper
Universität Paderborn, Paderborn, Germany

07.07.2016
Interaction and diffusion of solutes in Fe alloys: New insights from first principles
C. Fu
Service de Recherches de Métallurgie Physique, Saclay, France

14.07.2016
Engineering solutions for the conservation of cultural heritage
B. Wei
Rijksdienst voor het Cultureel Erfgoed, Amsterdam, The Netherlands

17.11.2016
Multiscale modelling of dislocation and plastic deformation in Magnesium and other HCP metals
Z. Wu
École Polytechnique Fédérale de Lausanne, Switzerland

08.12.2016
First-principles modelling of screw dislocation mobility in Zr and Ti
E. Clouet
Service de Recherches de Métallurgie Physique, Saclay, France

15.12.2016
Elastic strain engineering based on quantum-mechanical calculations
M. Friák
Academy of Sciences of the Czech Republic, Brno, Czech Republic

>> ICAMS Seminars and other Lectures 2015

19.03.2015
Phase diagrams from first principles using nested sampling
G. Csány
University of Cambridge, UK

22.04.2015
Cluster expansions for thermodynamics and kinetics of multi-component mixtures on fixed lattices
M. Sluiter
Delft University of Technology, The Netherlands

08.06.2015
High-throughput experimentation for discovery of solar fuels
S. K. Suram
California Institute of Technology, Pasadena, USA

16.06.2015
On the incorporation of environmental effects on multi-scale modelling approaches
E. Busso
ONERA - National Aerospace Research Centre, Palaiseau, France

16.06.2015
Scale hopping materials simulations and real atoms
D. Raabe
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

16.06.2015
From atoms to autos: Successes and challenges
W. Curtin
École Polytechnique Fédérale de Lausanne, Switzerland

16.06.2015
Monte Carlo study of Cu precipitation in Fe - From temperature-dependent cluster expansion to local chemical environment potentials
E. Kozeschnik
Technische Universität Wien, Austria

22.07.2015
Formation and growth of shear bands in glasses: Existence of an underlying directed percolation transition
J. Horbach
Heinrich Heine Universität, Düsseldorf Germany

21.09.2015
The design of magnetic materials with high spin polarization by first-principles
K. Yao, Z. Liu, G. Gao, L. Zhu
Huazhong University of Science and Technology, Wuhan, China

29.09.2015
Kinetic precipitation paths in solids
M. Bonvalet
Normandie Université, Saint Etienne du Rouvray, France

30.09.2015
More physics into Calphad modeling, finite temperature calculations, an example with the Fe-W system
A. Jacobs
Forschungszentrum Jülich, Germany

16.11.2015
A multi-scale perspective on grain boundary failure
C. Hüter
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

16.11.2015
Dipolar Bose-Einstein condensates with weak disorder
A. Pelster
Technische Universität Kaiserslautern, Germany

>> ICAMS Seminars and other Lectures 2016

05.02.2016
Including hydrodynamics and adaptivity in particle systems on parallel computers
G. Sutmann
Forschungszentrum Jülich, Germany

11.03.2016
Size effects in the mechanical behavior of nanoporous gold
K. Mangipudi
Georg-August Universität Göttingen, Germany

11.04.2016
A scalebridging approach to quantitatively link microstructure and machinability of steels
S. Münstermann, B. Wu
RWTH Aachen, Germany

02.05.2016
Development of high thermal conductivity steels
S. Weber
Bergische Universität Wuppertal, Solingen, Germany

02.05.2016
An industrial age for materials simulations
N. Marzari
École Polytechnique Fédérale de Lausanne, Switzerland

02.05.2016
Materials by design®: Developing and deploying novel high performance alloys using integrated computational materials engineering
N. Hatcher, J. Sebastian, J. Saal, G. B. Olson
QuesTek Innovations LLC, Evanston, USA and Northwestern University, Evanston, USA

02.05.2016
How useful is entropy maximization in structural materials design?
E. George
Ruhr-Universität Bochum, Germany

03.05.2016
Hidden pathway and defect generation during structural phase transformations
Y. Wang, Y. Gao
The Ohio State University, Columbus, USA

03.05.2016
Combinatorial and high-throughput methods for the design of new materials
A. Ludwig
Ruhr-Universität Bochum, Germany

13.05.2016
The influence of hydrogen on mechanical behavior of metallic materials
M. Mrovec
Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany

19.05.2016
Achieving room-temperature ductility for monolithic tungsten (W)
J. Reiser
Karlsruher Institut für Technologie, Germany

17.06.2016
Ultra-precision manufacturing of functional surfaces in advanced on-line/in-process surface inspection
Z. Tong, F. Gao
University of Huddersfield, United Kingdom

21.06.2016
Importance of inclusion of the effect of s electrons into bond-order potentials for transition bcc metals with d-band mediated bonding
V. Vitek
University of Pennsylvania, Philadelphia, USA

14.07.2016
Virtual testing of metallic materials: From nanomechanical testing to simulation of macroscopic properties
J. Llorca, J. Segurado
Universidad Politécnica de Madrid, Spain

06.09.2016
Designing CALPHAD-based thermodynamic models with open-source software
R. Otis
Pennsylvania State University, State College, USA

28.09.2016
ICME research at TCS and ICME enabling platform TCS PREMAP
P. Zagade, D. Khan
TCS Innovation Labs, Pune, India

31.10.2016
Micromechanical modelling of small scale plasticity: Strain gradient and field dislocation mechanics approaches
S. Gupta
University of Illinois, Urbana, USA

09.11.2016
Discrete kinetic theory: Lattices and entropy
S. Ansumali
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

Collaborations, Guests and Visitors

17. Collaborations, Guests and Visitors

>> Guests and visiting scientists 2015 and 2016

Dr. Santosh Ansumali
Jawaharlal Nehru Centre for Advanced Scientific Research
08.11.2016-09.11.2016

Dr. Livia Bartok-Partay
University of Cambridge
Cambridge, UK
19.03.2015-20.03.2015

Dr. Sonja Berghoff
Universitätsallianz Ruhr
Bochum, Germany
11.12.2015-31.12.2015, 01.01.2016-31.05.2016

Prof. Dr.-Ing. Erik Bitzek
Friedrich-Alexander-Universität Erlangen-Nürnberg
Erlangen, Germany
19.01.2015-21.01.2015

Manon Bonvalet
Normandie Université
Saint Etienne du Rouvray, France
29.09.2015

Sorcha Botwright
University of Oxford
Oxford, UK
09.07.2015-29.08.2015

Univ.-Prof. Dr.-Ing. Christoph Broeckmann
RWTH Aachen
Aachen, Germany
09.07.2015

Prof. Dr. Esteban Busso
ONERA - National Aerospace Research Centre
Palaiseau, France
16.06.2015

Dr. Emmanuel Clouet
Service de Recherches de Métallurgie Physique
Saclay, France
08.12.2016

Dr. Gábor Csány
University of Cambridge
Cambridge, UK
19.03.2015-20.03.2015

Prof. Dr. William Curtin
École Polytechnique Fédérale de Lausanne
Lausanne, Switzerland
16.06.2015

M.Sc. Theresa Anne Davey
Imperial College
London, UK
06.01.2015-14.01.2015, 23.09.2015-30.09.2015, 08.02.2016-23.02.2016, 08.08.2016-20.08.2016

M.Sc. Maarten De Jong
University of California, Berkeley
Berkeley, USA
07.09.2015-31.12.2015, 01.01.2016-01.04.2016, 14.04.2016-21.04.2016

Prof. Dr.-Ing. Karsten Durst
Technische Universität Darmstadt
Darmstadt, Germany
04.02.2016

Simen Eliassen
University of Oslo
Oslo, Norway
05.10.2015-29.10.2015

Prof. Dr. Michael Finnis
Imperial College
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Teaching and Lectures

18. Teaching and Lectures

2015

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Application and implementation of electronic structure methods

S. G. Fries
The CALPHAD method

T. Hammerschmidt, R. Janisch, J. Rogal
Interfaces and surfaces

A. Hartmaier
Microstructure and mechanical properties

I. Steinbach, F. Varnik, O. Shchyglo
Phase-field theory and application

R. Drautz
Quantum mechanics in materials science

>> MSS lecture courses winter term 2015/16

J. Rogal
Advanced atomistic simulation methods

R. Drautz
Atomistic simulation methods

R. Janisch, Y. Motemani
Assessment and description of material properties

I. Steinbach
Continuum methods in materials science

R. Drautz, R. Janisch, M. Piacenza
Documenting and communicating science

V. Yardley, G. Eggeler
Elements of microstructure

T. Hickel
Introduction to quantum mechanics in solid-state physics

F. Varnik
Lattice Boltzmann modeling: From simple flows to interface driven phenomena

E. George
Materials processing

A. Hartmaier, A. Ma
Modelling of metal plasticity in finite element analysis

A. Hartmaier, T. Hammerschmidt
Multiscale modelling in materials science

A. Hartmaier
Numerical simulation of fracture of materials

I. Steinbach, O. Shchyglo, F. Varnik
Phase-field theory and application II: Advanced techniques and miscellaneous problems

G. Madsen, C. Begau
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Solidification processing

R. Darvishi Kamachali, F. Varnik
Statistical physics and thermodynamics

>> Other courses

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Introduction to modelling in materials science

>> SurMat *Multiscale Modelling*, 23.-27.02.2015

R. Drautz
Atomic interactions and dynamics

T. Hammerschmidt
Calculation of material properties

A. Hartmaier
Continuum solid mechanics and finite element method

J. Neugebauer
Fundamentals of ab initio simulations and their application to surface physics

I. Steinbach
Microstructure evolution and phase transitions

A. Hartmaier
Modeling multiphase materials

A. Hartmaier
Models for microstructure properties relations

I. Steinbach
Moving boundary problems

I. Steinbach
Phase field method

T. Hammerschmidt
Setup and analysis of molecular dynamics simulations

2016

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R. Drautz, J. Neugebauer
Application and implementation of electronic structure methods

S. G. Fries
The CALPHAD method

T. Hammerschmidt, R. Janisch, J. Rogal
Interfaces and surfaces

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Microstructure and mechanical properties

I. Steinbach, F. Varnik, O. Shchyglo
Phase-field theory and application

R. Drautz
Quantum mechanics in materials science

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Advanced atomistic simulation methods

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Assessment and description of material properties

R. Drautz
Atomistic simulation methods

A. Hartmaier
Computational fracture mechanics

I. Steinbach
Continuum methods in materials science

R. Drautz, R. Janisch, M. Piacenza
Documenting and communicating science

G. Eggeler
Elements of microstructure

T. Hickel
Introduction to quantum mechanics

F. Varnik
Lattice-Boltzmann modeling: From simple flows to interface driven phenomena

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Materials processing

A. Hartmaier, T. Hammerschmidt
Multiscale modelling in materials science

G. Sutmann, T. Hammerschmidt
Programming concepts in materials science

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Solidification processing

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Statistical physics and thermodynamics

A. Hartmaier, N. Vajragupta
Theory and application of micromechanical modelling

>> SurMat *Multiscale Modelling*, 22.-26.02.2016

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J. Rogal
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T. Hammerschmidt
Simulation of STM experiments

O. Shchyglo
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Calphad method with practical exercises

F. Varnik
Lattice Boltzmann modeling of multiphase flows

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