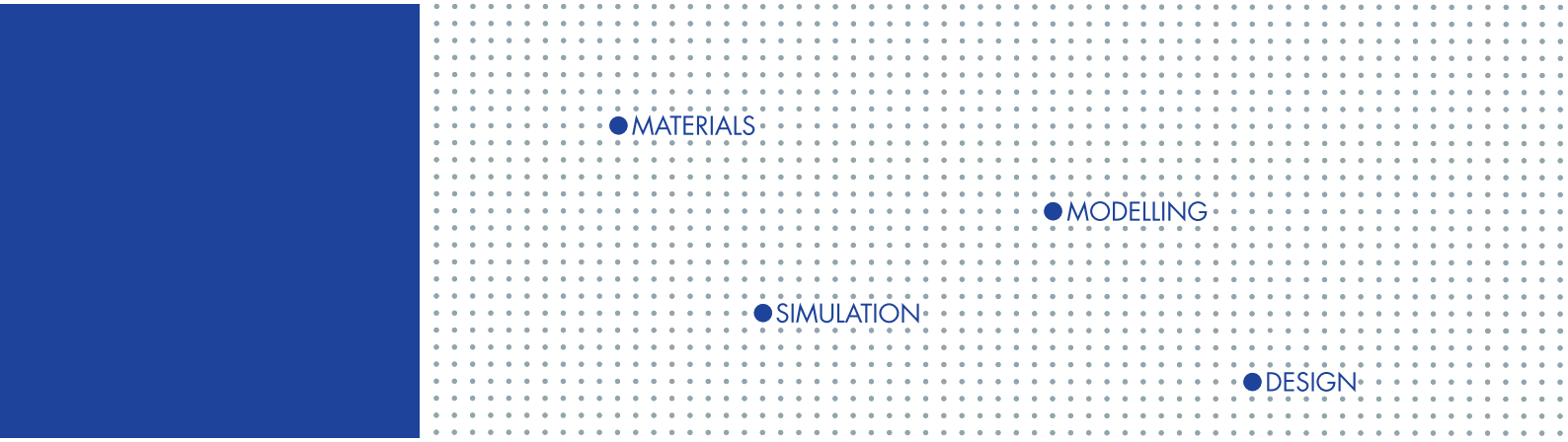
Scientific Report 2017 and 2018



ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS

Scientific Report 2017 and 2018

ICAMS
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Universitätsstr. 150
44801 Bochum
Germany

Preface

The 10th anniversary of ICAMS was celebrated in 2018 with a scientific symposium visited by internationally leading materials scientists[1]. Since its start, ICAMS grew into a worldwide recognized centre for materials modelling that complements the strong experimental materials science activities on the campus of Ruhr-Universität Bochum.

Fig. 1: Participants of the 10 Years ICAMS symposium.

We would like to take this opportunity to thank everybody who contributed to making ICAMS a success: Ruhr-Universität Bochum together with all our colleagues, who continuously supported us; our partners from industry, who provided inspiration for current research topics of industrial relevance and generous start-up funding; the state of North-Rhine Westphalia and the European Union, who complemented this funding; the funding agencies, in particular Deutsche Forschungsgemeinschaft, which made our work possible; the members of our academic and industrial advisory board, who helped us to shape ICAMS; all our research partners worldwide; and – last, but absolutely not least – the present and past members of ICAMS, who dedicated their energy and ingenuity to advance materials modelling and simulation.

Alexander Hartmaier
Managing Director

Ingo Steinbach
Director

Ralf Drautz
Director

[1] The views and ideas of some participants of the symposium, some of whom had accompanied ICAMS from its very start, are documented in a short video.

Contents

ICAMS

ICAMS in 2017 and 2018

2. ICAMS in 2017 and 2018

2018 marked the 10th anniversary of ICAMS. Leading international scientists attended our 10 Years ICAMS symposium and contributed to make it a truly remarkable event. The role of ICAMS as a world leading centre for scale-bridging materials modelling was widely acknowledged.

ICAMS ramped up its activities in the quickly evolving field of data-oriented science. As a first step, the ICAMS retreat in 2018 had been devoted to this topic. Subsequently, ICAMS established a tenure track junior professorship "Materials Informatics and Data Sciences", which is currently being filled.

The following sections provide a summary of the ICAMS activities.

► 10 Years ICAMS

In 2018 we celebrated the 10th anniversary of our institute with an international symposium. The aim of the three-day meeting was to highlight cutting edge developments in the rapidly growing field of scale-bridging materials modelling and to bring together internationally leading scientists in the field. Ten international experts (see box) gave invited talks during the symposium. Furthermore, 40 contributed talks and 40 posters gave an overview of one decade of scale-bridging materials modelling.

Mark Asta
University of California, Berkeley, USA

Irene Beyerlein
University of California, Santa Barbara, USA

Long-Quing Chen
Penn State, State College, USA

Bill Curtin
EPFL, Lausanne, Switzerland

Antonín Dlouhý
IPM, Czech Academy of Sciences, Brno, Czech Republic

Dennis Kochmann
ETH Zurich, Switzerland

Javier Llorca
Technical University of Madrid, Spain

Greg Olson
QuesTek Innovations LLC
and Northwestern University, Evanston, USA

Eugen Rabkin
Technion, Haifa, Israel

Cynthia Volkert
Universität Göttingen, Germany

Recent progress in bridging the gap between academic and industrial research and application of multiscale modelling for materials design was addressed in a plenary discussion "Skalenüberbrückende Materialsimulation: Gestern, heute und morgen", with keynote speakers and participants from academia, industry and politics.

Fig. 2.1: Impressions from the 10 Years ICAMS symposium in June 2018.

▸ Workshops and Conferences

ICAMS organised and contributed to the organisation of several workshops and conferences in the past two years. In March 2017 the international workshop and tutorial series "Modelling and Simulation of Superalloys" took place.

The ICAMS Advanced Discussions in May 2017 were dedicated to High performance computing and industry. Speakers from industry and research institutions were complemented by oral and poster contributions from ICAMS. The symposium "Bonding and Structure in Materials" to celebrate and honour the life and work of the late Professor David Pettifor CBE FRS at the University of Oxford was co-organized by ICAMS. In August 2018 the Sino/German symposium and workshop "Material-Oriented Micro/Nano Manufacturing: Modelling, Experiment and Application" took place in Bochum and like every other year, the ASG Modelling and the AMS department organized the ADIS workshop at Ringberg castle. ICAMS lead the organisation of the 2018 Materials Chain conference in Bochum.

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

- Data Driven Materials Design, symposium at the DPG spring meeting Dresden, 2017
- Mechanical Properties and Mechano-Chemical Coupling, symposium at the DPG spring meeting Dresden, 2017
- Emergent Material Properties and Phase Transitions under Pressure, symposium at the MRS spring meeting, Phoenix, 2017
- CALPHAD XLVI, Saint-Malo, 2017
- Magnetism in Materials Science, symposium at the DPG spring meeting Berlin, 2018
- CALPHAD XLVII, Querétaro, 2018
- International Workshop on Co-base Superalloys 2018, London, 2018
- TOFA 2018, Seoul, 2018
- Topic coordination “Modelling and Simulation” and symposia, MSE, Darmstadt 2018

▸ Teaching

ICAMS regularly organises excursions to bring the students of its international master’s programme “Materials Science and Simulation” into contact with companies in Germany. The 2017 excursion led us to the Stuttgart area, where we visited a production unit of Daimler AG, the research campus of Robert Bosch GmbH, the R&D department of Anton Paar GmbH as well as the Max Planck Institute for Intelligent Systems and the University of Stuttgart, in addition to a number of social activities. In 2018 our students visited Berlin, including a stop in Wolfsburg and a tour of the production at Volkswagen. In Berlin, we saw the Siemens turbine production and enjoyed visits to Atotech, BAM and Bessy.

From 2017 to 2018 the number of applicants for our master’s programme “Materials Science and Simulation” increased from around 454 to 686. 59 students were admitted in 2017 and 64 in 2018. Altogether 50 students eventually took up their studies in the last two years. 15 master’s students successfully graduated in 2017 and 24 in 2018.

At ICAMS, we currently explore new possibilities for teaching that are offered by electronic media to support learning processes and improve interactions with students.

Fig. 2.2: Excursion of our master students to Berlin in 2018.

Regular "fireplace talks" at which former graduates from ICAMS present their view and experience about their job and career prospects in a relaxed and informal atmosphere further facilitate interactions between ICAMS students and industry.

Three inaugurational lectures were given on 17th October 2017. Rebecca Janisch successfully completed her habilitation with the inaugurational lecture. Godehard Sutmann and Fathollah Varnik, who had been appointed as professors in 2017, introduced themselves formally to ICAMS.

Fig. 2.3: ICAMS Fireplace talks. Top: Jörg Koßmann (Clouth Sprenger) and Philipp Engels (Siemens AG), bottom: Sebastian Schreiber (thyssenkrupp Steel Europe AG) and Anika Marusczyk (Robert Bosch GmbH).

Fig. 2.4: Fathollah Varnik, Rebecca Janisch and Godehard Sutmann (from left to right) after the inaugural lectures in October 2017.

► Staff numbers

While ICAMS staff numbers were nearly constant in 2017 and 2018, ICAMS plans to expand in the near future. ICAMS will establish several new groups and hire further scientists in 2019 and we expect that the number of researchers at ICAMS will be between 80 and 90. In 2017 and 2018, about three quarters of the ICAMS staff where 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, 85% of the acquired third party funds came from public funding agencies, primarily from Deutsche Forschungsgemeinschaft, and 15% from industry.

► Publications

In 2017 and 2018, ICAMS researchers, including researchers at the ICAMS Advanced Study Groups, published 166 papers. Furthermore, 12 theses have been completed by our PhD students and 48 Master theses were supervised or co-supervised in 2017 and 2018. *Figure 2.5* shows the number of publications since 2008. A detailed list of all publications from the last two years can be found in chapter 14.

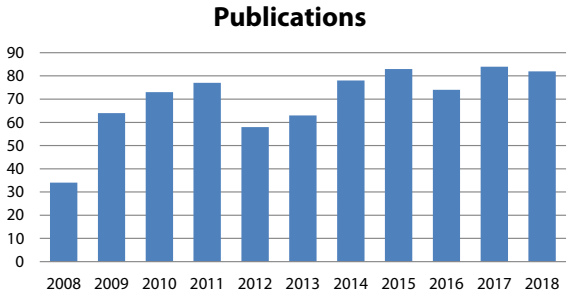

Fig. 2.5: ICAMS publications since 2008.

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Organisation of ICAMS

1. Organisation of ICAMS

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ICAMS

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 of Atomistic Modelling and Simulation works on the finest, most fundamental length scale of atomistic simulations.

Our research has three main objectives:

1. to obtain effective interatomic interactions from fundamental theories of the electronic structure;

2. to employ effective interatomic interactions in large scale and long-time atomistic simulations for obtaining effective models and parameters that may serve as input for the modelling activities of the two other ICAMS departments;

3. to develop data-driven and high-throughput atomistic simulation methods for model validation and the discovery of novel materials.

Interatomic potentials are obtained by systematically coarse graining density functional theory to effective models of the interatomic interaction. Potentials are employed in atomistic simulations for predicting structural stability and mechanical properties of materials and in rare event dynamics for modelling kinetics of phase transformations. In this way a coherent link from the electronic structure to the continuum description of materials on the meso- and macroscale is obtained.

Automated workflows together with high-throughput calculations are used to explore the chemical phase space of binary and ternary compounds, to validate trends in structural stability that are predicted by simplified models and for a systematic analysis of interatomic potentials.

Density functional theory calculations and statistical machine learning are employed for computational materials design and assist and guide experimental research. High-throughput density functional calculations further help to improve and reparameterise thermodynamic databases.

▸ Structure

Four research groups represent the department's focus on establishing a coherent link from the electronic structure through atomistic simulations to meso- and macroscopical modelling hierarchies.

- Atomistic simulation of structural and phase stability (Dr. Thomas Hammerschmidt)
- Atomistic simulation of mechanical behaviour (Dr. Matous Mrovec)
- Atomistic simulation of the kinetics of phase transformations (Dr. Jutta Rogal)
- Data-driven methods for atomistic simulations (Dr. Yury Lysogorskiy)

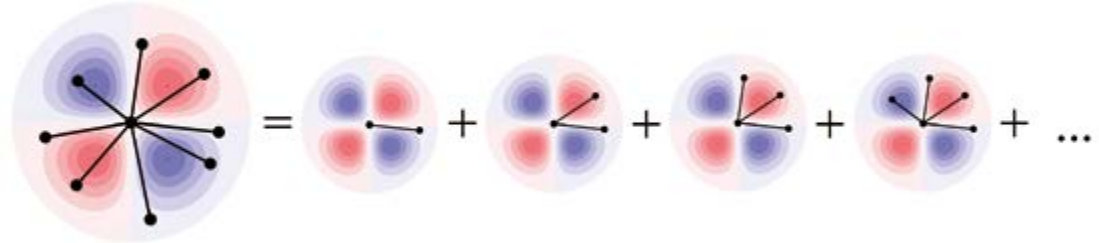


Fig. 4.1: Illustration of the atomic cluster expansion.

AMS

4.1. Atomistic Simulation of Structural and Phase Stability

Group leader:
Dr. Thomas Hammerschmidt

Group members:
Dr. Jan-Michael Albina
Dina Alfaouri
Dr. Miroslav Čák
Marc Densow
Jan Jenke
Dr. Alvin N. C. Ladines
Aparna P. A. Subramanyam
Ning Wang

▸ Research

The goal of the research group is to understand and optimise the properties of functional materials and to discover new materials by atomistic modelling and simulation. This requires adequate approaches to treat the diversity of the chemical composition (e.g. multi-component superalloys), the complexity of the microstructures (e.g. dislocations and precipitates in steels) and the complexity of the physical phenomena (e.g. magnetic phase transition in iron, finite-T properties of battery materials, dislocations in high-entropy alloys).

In our portfolio of materials-science methods, we combine density functional theory (DFT) as accurate small-scale method, tight-binding (TB) and analytic bond-order potentials (BOPs) as approximate large-scale methods as well as structure maps as complementary data-driven method. The TB and BOP models are obtained by a coarse-graining of the electronic structure that preserves the quantum-mechanical nature of the chemical bond. The analytic BOP allow us to perform large-scale atomistic simulations that capture the complexity of microstructure and physical phenomena. They also provide electronic-structure based descriptors of the local atomic environment that are applied in machine-learning of material properties. The highly predictive structure maps chart the bonding chemistry of known compounds with physically intuitive descriptors and enable us to predict structural stability in multi-component alloys.

▸ Competences

- Analytic bond-order potentials and tight-binding
- Structure maps of d-d and p-d valent systems
- High-throughput density functional theory calculations
- Descriptors of local atomic environments and machine learning
- Structural stability, point defects and interfaces in transition metal compounds

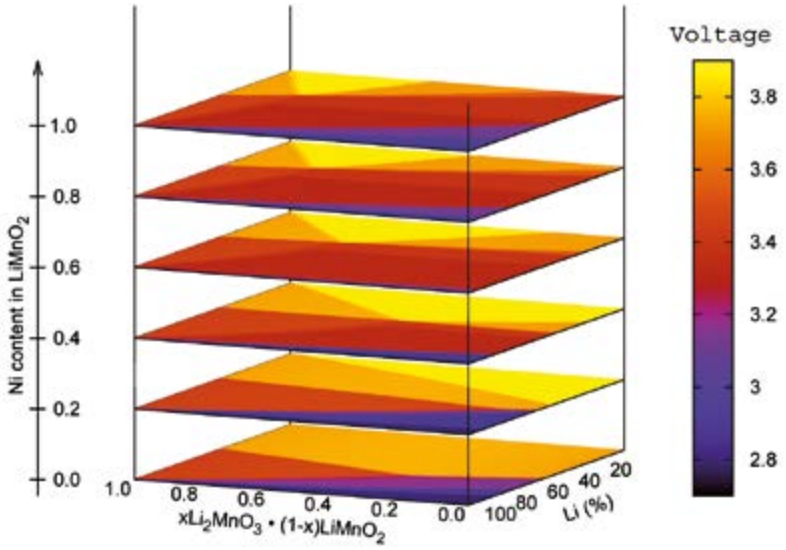


Fig. 4.2: Change of open circuit voltage of Li-Mn-Ni-O cathode material with concentration of Li and Ni at room temperature. This property map is based on density functional theory calculations of structural stability at T=0K that are upscaled in temperature by phonon calculations.

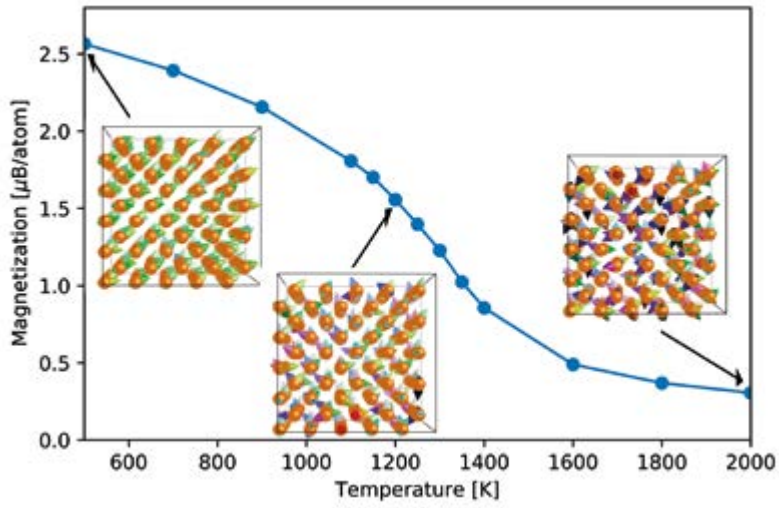


Fig. 4.3: Magnetisation of bcc-iron as a function of temperature obtained with a bond-order potential including non-collinear magnetism. The spin directions in the snapshots at 500K, 1200K, and 2000K indicate the collapse of the long-range and short-range magnetic order with increasing temperature.

AMS

4.2. Atomistic Simulation of Mechanical Behaviour

Group leader:
Dr. Matous Mrovec

Group members:
Tapaswani Pradhan
Matteo Rinaldi
Malte Fritz Schröder
Dr. Daria Smirnova
Dr. Sergei Starikov

▸ Research

The primary goal of the research group is to understand phenomena occurring on the atomic scale that are related to macroscopic mechanical behaviour. We start with 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 these with prototypical metallic and covalent chemical bonding as well as 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
- Magnetism

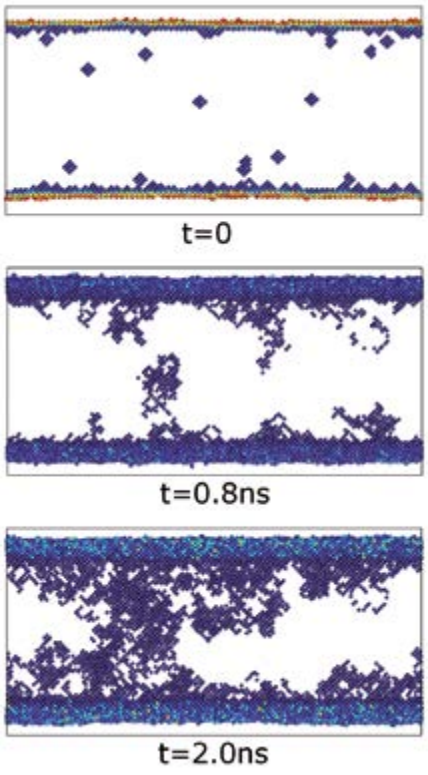


Fig. 4.4: Snapshots from molecular dynamics simulation of self-diffusion in Mo.

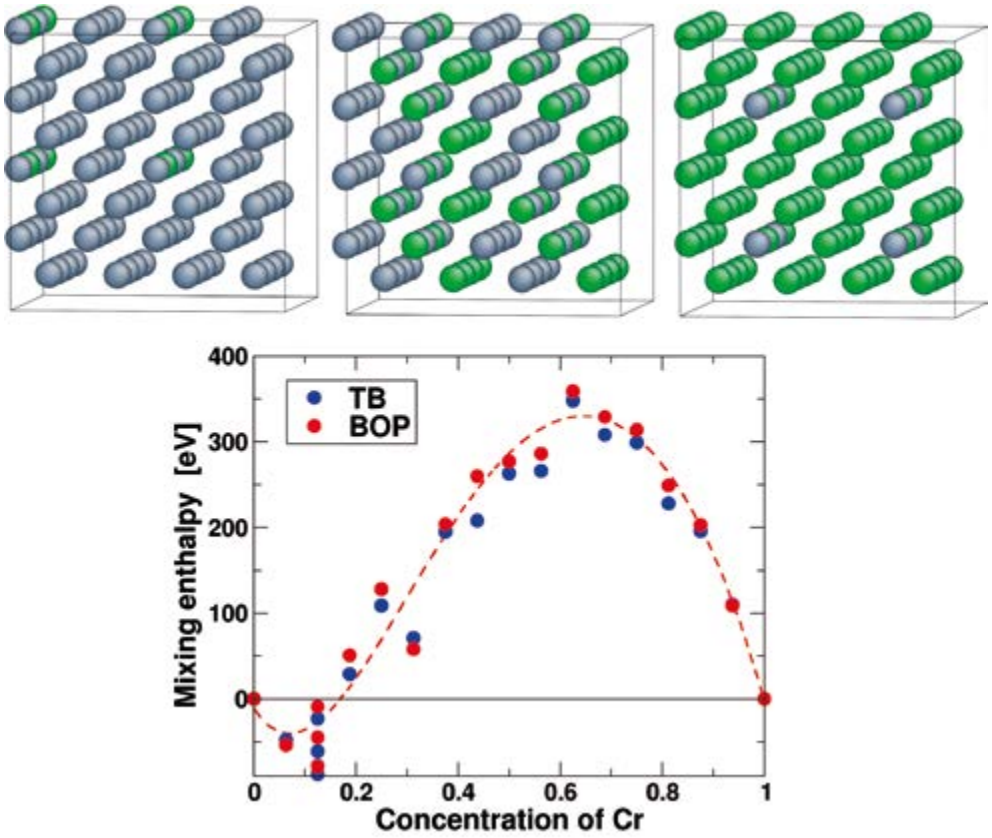


Fig. 4.5: Enthalpy of mixing for the Fe-Cr system predicted by BOP and TB models.

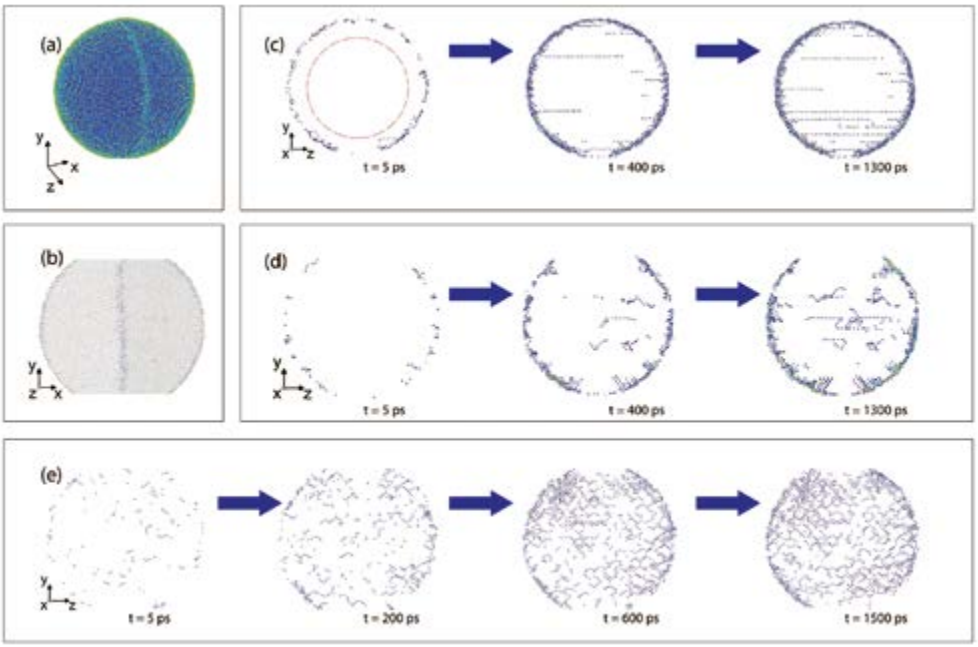


Fig. 4.6: Atomistic simulation studies of grain boundary (GB) diffusion. Simulated nanoparticle containing two misoriented bi-crystals (a, b); traces of diffusing atoms at a symmetric (c), asymmetric (d), and general (e) GB as function of time.

AMS

4.3. Atomistic Simulation of the Kinetics of Phase Transformations

Group leader:
Dr. Jutta Rogal

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

▸ Research

The central research objective of our group is the development and application of atomistic simulation techniques to characterise structural phase transformations in technologically relevant materials. Applications range from high-performance to functional materials such as single crystal superalloys or high-temperature shape memory alloys. Phenomena of interest include atomistic diffusion and the mobility of point defects, martensitic transformations, the initial stages of nucleation and growth, and phase boundary migration. An atomistic description of these dynamical processes is particularly challenging since the involved timescales go far beyond the application range of classical molecular dynamics simulations and require the use of advanced simulation techniques.

Our recent research highlights include: The investigation of composition dependent vacancy mobilities in binary Ni-X (X=Re, W, Ta) alloys using a combination of highly accurate electronic structure calculations and kinetic Monte Carlo simulations; the prediction of ternary Ti-Ta-X alloys with high transformation temperatures from first-principles data; the characterisation of martensitic transformations in Ti-Ta on the basis of ab initio molecular dynamics; the quantitative evaluation of reaction coordinates for nucleation and growth during solidification in Ni combining transition path sampling and a maximum likelihood estimation; transition path sampling of heterogeneous nucleation and chemical ordering during nucleation in binary Ni-Al alloys.

▸ Competences

- Nucleation, growth, and phase transformation diffusion
- (Adaptive) Kinetic Monte Carlo
- Enhanced sampling techniques
- Transition path sampling

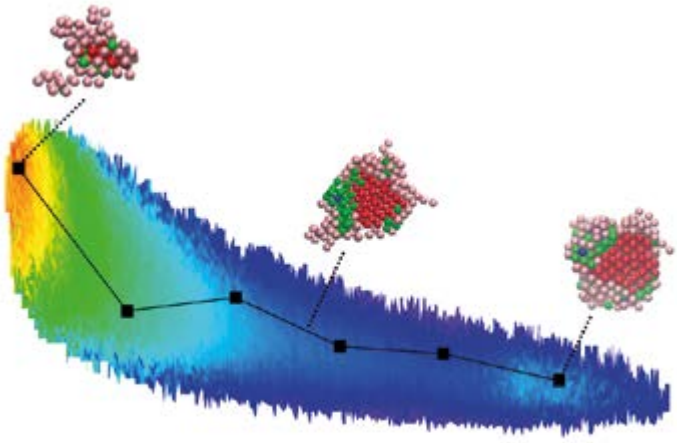


Fig. 4.7: Free energy landscape and optimal reaction coordinate for nucleation in Ni; the initial stage of the nucleation process is characterised by the formation of a precursor zone in the undercooled liquid before the crystal structure emerges from this preordered region; red spheres are fcc atoms, green hcp atoms, and light-brown are prestructured atoms.

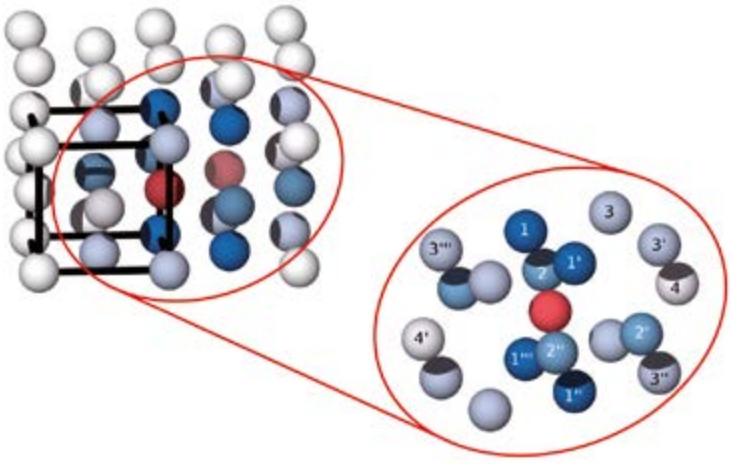


Fig. 4.8: Diffusion channel for a nearest neighbour jump process in an fcc lattice; the diffusion barrier depends on the occupation of the diffusion channel with solute and host atoms; the diffusion channel (blue atoms) contains all first-nearest neighbours to the initial and final position of the diffusing atom (red); the different shades of blue and the labelling indicate the distance from the transition state.

AMS

4.4. Data-Driven Methods for Atomistic Simulations

Group leader:
Dr. Yury Lysogorskiy

► Research

The research group is working on the application of data-driven methods in materials science with a particular focus on the atomic scale. A major research area is the automated extraction, analysis and validation of models in materials science, with specific application to interatomic potentials. We perform high-throughput calculations of materials properties at different levels of theory, including both density functional theory and effective interatomic potentials using the pyiron computational framework, which we co-develop with the Computational Materials Design department at the Max Planck Institute für Eisenforschung.

Another research area is the application of machine learning methods to large data sets, for example, from combinatorial or high-throughput methods and to provide efficient and supporting tools for materials discovery.

► Competences

- Data-driven methods (incl. machine learning) in materials science
- High-throughput calculations (DFT and molecular dynamics)
- Interatomic potentials and their validation
- Data management and visualisation

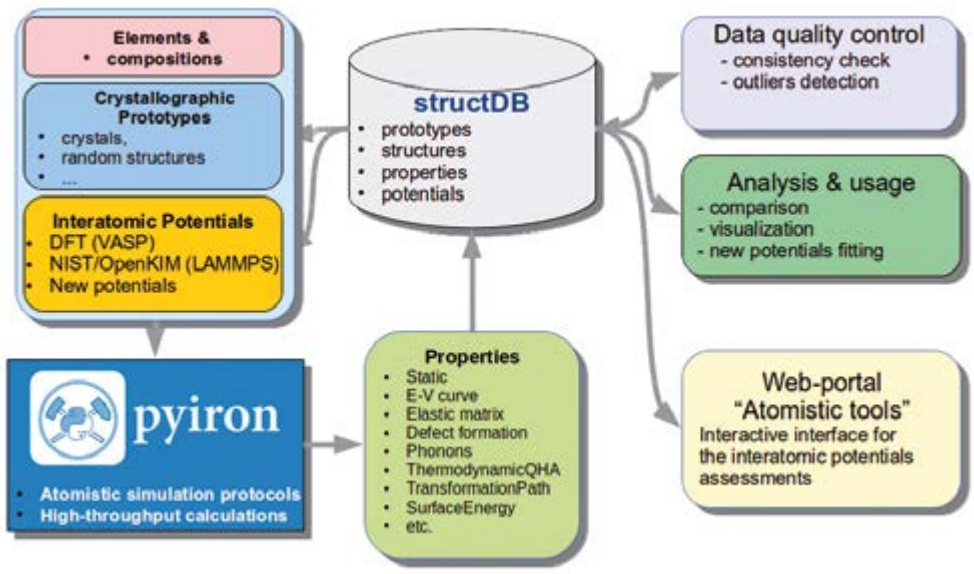


Fig. 4.9: Computational and data infrastructure for interatomic potentials validation.

ICAMS

Department Scalebridging Thermodynamic and Kinetic Simulation STKS

5. Department Scalebridging 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 analyse 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. A new activity is data mining and statistical analysis of materials data, based in the junior research group of Dr. Irina Roslyakova. The start-up OpenPhase solutions GmbH was founded with the long-term goal of maintaining the development of the phase-field software OpenPhase in an academic environment, and to provide services to industrial and academic customers.

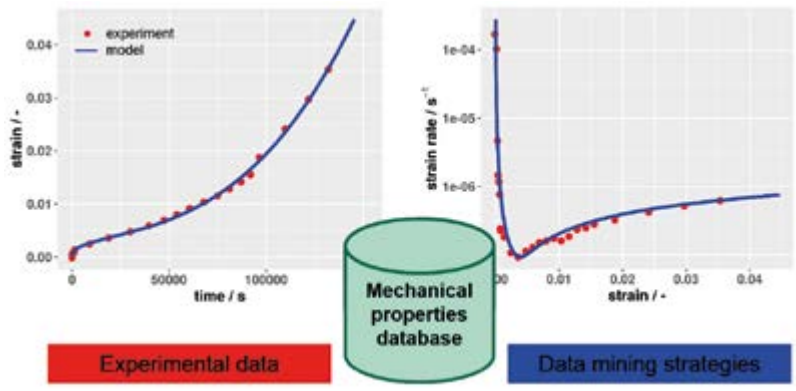


Fig. 5.1: Mechanical properties experimental and modelling database.

▸ Structure

The department's activities are organised in four groups, focusing 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 (Prof. Dr. Fathollah Varnik)
- Data Mining and Statistical Analysis (Dr. Irina Roslyakova)

5 PhD theses and 17 master theses have been completed during the last two years. 12 doctoral projects are currently on-going at STKS.

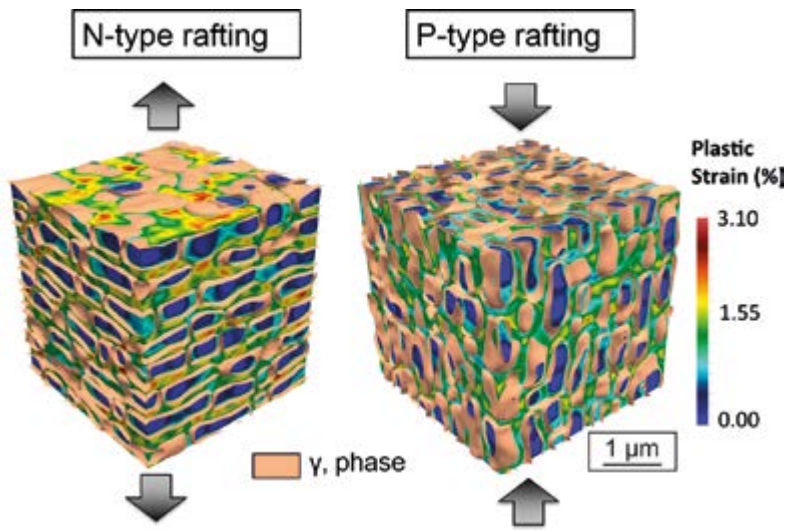


Fig. 5.2: Rafting of a Ni-base superalloy under uniaxial tensile or compressive load in the high temperature-low stress regime; by coupled phase-field/crystal plasticity simulation.

STKS

5.1. Computational Thermodynamics/CALPHAD

Group leader:
Dr. Suzana G. Fries

▸ Research

The goal of the group is to incorporate first-principles calculated quantities into thermodynamic modelling of Gibbs energies of stable and metastable phases following the CALPHAD method which is mainly based on experimental observation. These data can be used to understand material behaviour, optimise processes, improve materials properties and support its design. The different levels of the use require of the data require a fluent transfer of information, and the group is engaged to follow the protocol established by the Integrated Computational Materials Engineering (ICME) effort. The very close contact with communities developing materials like Ni-Co based superalloys, steels, multi-principal elements alloys, Ti-alloys etc, at ICAMS, at RUB, in the country and internationally, gives the group the possibility to directly observe the demands of the developers. Realising the necessity of having data with a high level of predictability but kept compact in order to not overload simulations, a model called Effective Bond Energy Formalism was recently created in cooperation with external researchers. The enthalpies of formation for binary end-members of complex phases (e.g. σ, μ, Laves) calculated using functional density theory (DFT) are used to predict ternary phases behaviour with an accuracy not very different from the one obtained by ternary calculations done with DFT (which can be obtained by the interaction with AMS). A huge number of open databases is added to the collection of own thermodynamic assessments. The possibility to have access to model parameters allows not only to see trends in phase stability but also to support modelling of systems that are not yet evaluated thermodynamically.

▸ Competences

- Thermodynamic modelling
- Order-disorder solid solutions
- Open Calphad library development
- Critical evaluation of experimental data relevant to thermodynamic modelling
- ICME

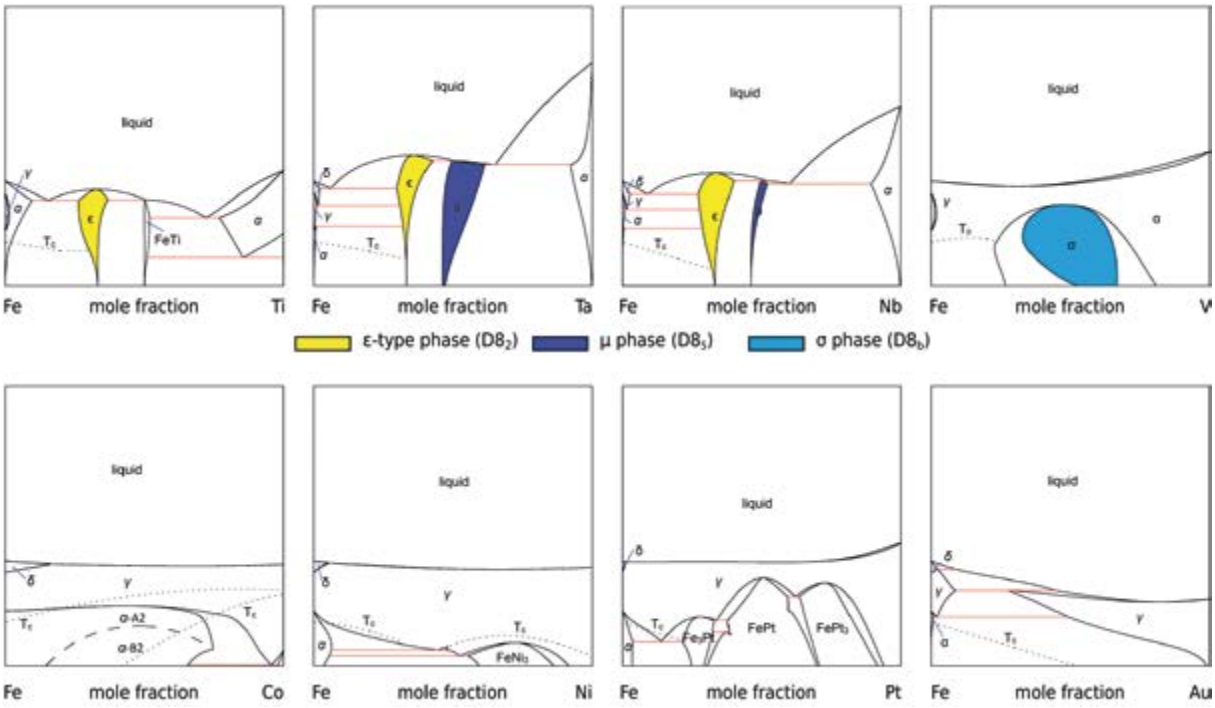


Fig. 5.3: Following the sequence of the Mendeleev number M, proposed by D. Pettifor (Figure 5.4), Fe-M binary diagrams are arranged in the first sequence for M=51 to 54, and in the sequence bellow for M=64 to 70. D82, D8b and D85 phases are highlighted to indicate the similarities of the phase diagrams.

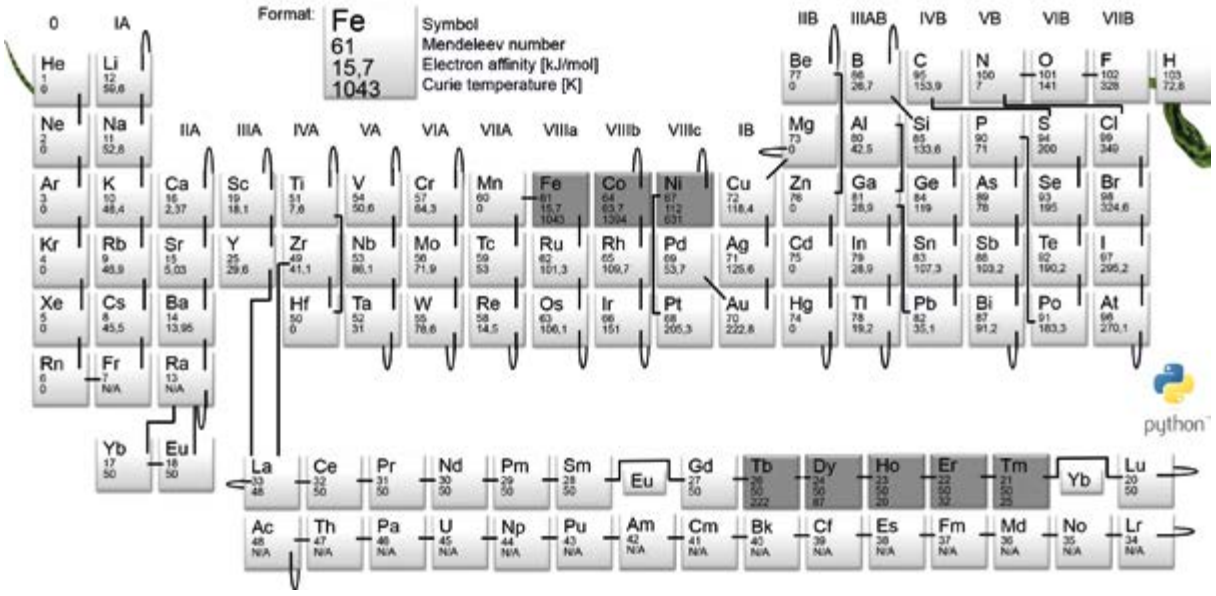


Fig. 5.4: The snake running through this modified periodic table is following the Mendeleev number (D. G. Pettifor, Solid State Communications 1984).

5.2. Phase-Field Simulations of Microstructures

Group leader:
Dr. Oleg Shchyglo

Group members:
Katrin Abrahams
Muhammad Adil Ali
Dr. Johannes Viktor Görler
Stephan Hubig
Dr. Julia Kundin
Hesham Salama
Matthias Stratmann

▸ Research

Our research group focuses on the development of new methods for phase-field simulations of micro-structures in complex materials. At present, the range of applications for phase-field modelling includes solidification, grain growth, eutectic and peritectic reactions, recrystallisation, and martensitic transformations. If one wants to make a quantitative prediction 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 energies is widely available in databases, the free energy contributions from elasticity and plasticity data is not easily available. Our goal is not only to provide a reliable simulation platform for phase-field simulations, but also to provide free energy contributions which are at present omitted in the thermodynamic databases. In collaboration with the 'CALPHAD Thermodynamics' group, we develop the free energy models, which incorporate 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 modeling
- Phase transformations
- Microscopic elasticity theory
- "OpenPhase" library development

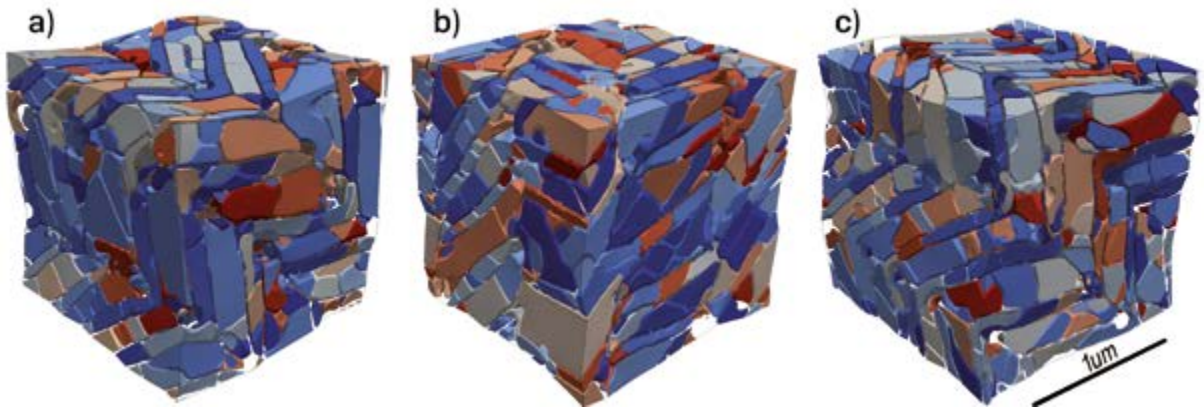


Fig. 5.5: Simulated martensite microstructure of steel for different carbon content: (a) 0.1% (b) 0.2% and (c) 0.3%.

5.3. Theory and Simulation of Complex Fluids

Group leader:
Prof. Dr. Fathollah Varnik

Group members:
Marian Bruns
Muhammad Reza Hassani
Dr. Alexandra Lagogianni
Elias Mahmoudinezhad
Raphael Schiedung
Samad Vakili
Dr. Marvin Tegeler
Haifeng Wang

▸ Research

Research interests of the group cover a rather broad range of physical problems including fluid structure interactions, wetting and capillarity in granular media, phase transformations kinetic and deformation behaviour of amorphous materials.

Recently, a particular focus of the complex fluids group has been on molecular dynamics simulation studies of glass forming metallic alloys and the growing range of spontaneous strain-correlations upon cooling. The connection between these correlations and the closely related emerging elasticity with shear banding and brittle failure in metallic glasses is one of the major research topics of the group.

Another area of activity within the group is mesoscopic modelling of liquid phase sintering. This is a multi-physics problem, which includes phase transformation and microstructure evolution in wet granular powders under the action of capillary forces, the resulting particle rearrangements and mass transport in the liquid phase.

Molecular dynamics studies of shape memory polymers are another topic actively addressed by the group. A main goal here is gaining a better understanding of the effect of additive small molecules on the recovery temperature and their potential as a switching parameter to trigger shape recovery.

▸ Competences

- Modelling multiphase flows
- Mechanical response of amorphous materials
- Molecular dynamics of polymers
- Hybrid lattice Boltzmann phase-field modelling

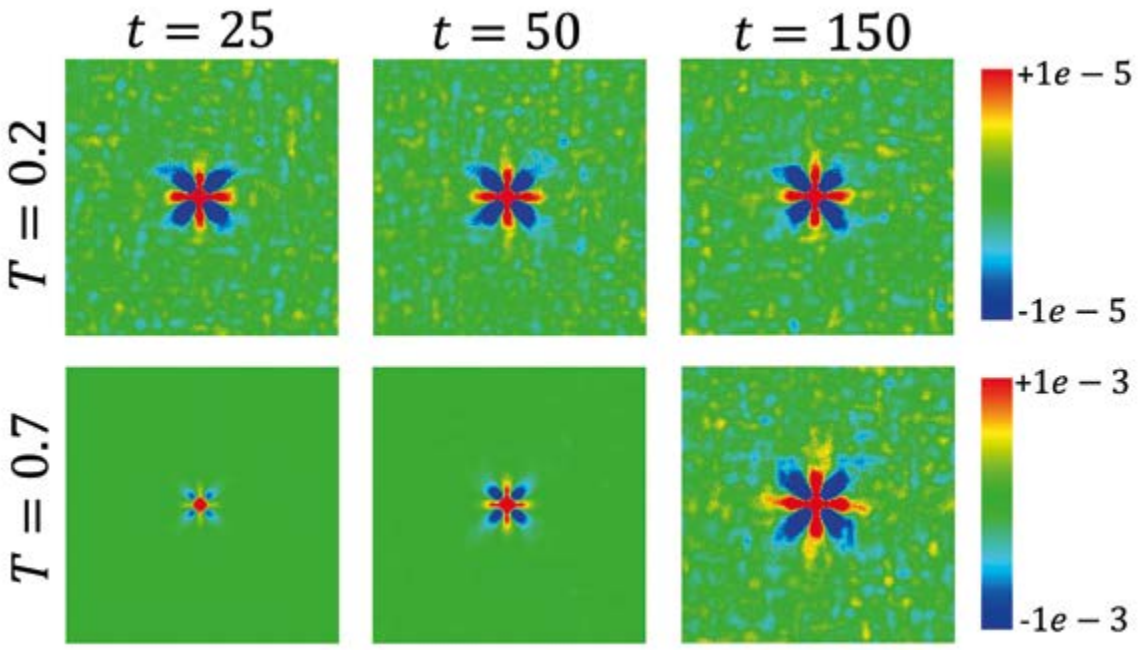


Fig. 5.6: Spatial correlations of spontaneous (non-affine) strain in a model metallic glass. Note first of all the striking similarity to the Eshelby pattern around a pre-sheared spherical inclusion both in the solid (upper row) and in the liquid (lower row) states. Each non-affine particle strain event thus seems to play the role of an inclusion in the spirit of the Eshelby-problem. This has been recently rationalised quantitatively within a generalised hydrodynamics theory [Hassani et al, Europhys. Letters 124, 18003 (2018)]. Moreover, we have also shown that this analogy is general and holds also close to hard boundaries, where the four-fold symmetry is broken [Hassani et al, Europhys. Letters 121, 18005 (2018)]. The spontaneous strain is obtained as gradient of the particles' displacements within time t. In the solid (upper row), particles have already explored their immediate neighbourhood, but cannot go beyond. Therefore, the amplitude of correlations remains stationary. In the supercooled state, on the other hand, particles continue exploring ever larger domains with time, leading to a growth of the correlation amplitude (note the difference in scale bars).

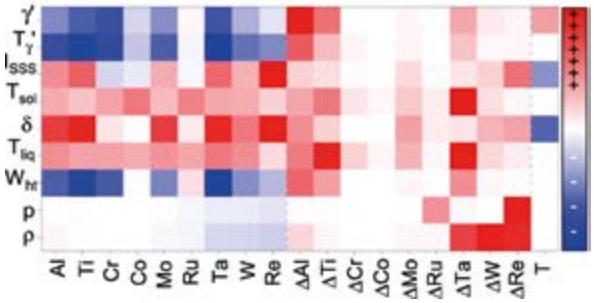
5.4. Data Mining and Statistical Analysis

Group leader:
Dr. Irina Roslyakova

Group members:
Abdulmonem Obaied
Setareh Zomorodpoosh

▸ Research

The group works on the development of data-driven and physically-based modelling strategies and their application to analysis and interpretation of materials data. At the moment, one of the key research topics is the development of physically-based and data-driven models to identify statistically sound correlations between materials chemistry, thermodynamic, microstructure and mechanical data of single crystal Ni- and Co-based super alloys. In comparison to the existing purely phenomenological modelling methods, such hybrid modelling strategies allow to identify the influence of individual physical effects from the considered contribution on selected material properties. Moreover, they are frequently required to accelerate the computer-based design of new materials and alloys, for example, the development of rhenium-free Ni-based alloys with desirable mechanical properties.



Due to the high complexity and heterogeneity of materials data, we focus mainly on three key goals:

- the establishment of a well-organised data infrastructure for storage of experimental data and simulation results;
- the development of robust physics-based models of materials properties and their application for thermodynamic calculations and integration into computer-based alloy-by-design framework;
- the development and application of data mining and machine learning methods to identify statistically sound correlations between materials chemistry, microstructure and mechanical data.

Moreover, a combination of this modelling technique and the application of statistical design of experiments allow to reduce the number of experimental trials required for the development of new materials and processes.

Fig. 5.7: Normalized standardized regression coefficients of alloying elements and their variations in at% for property variation within a full linear regression model.

► Competences

- Material informatics incl. data mining and machine learning methods
- Automation of data and image processing
- Development of physics-based materials properties models
- Mathematical third generation CALPHAD databases: mathematical aspects
- Design of experiments

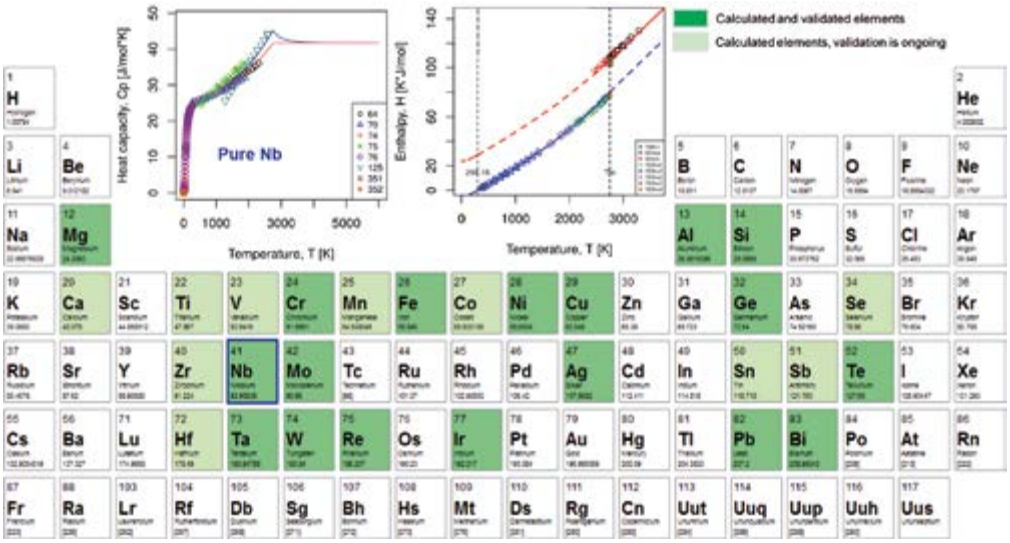


Fig. 5.8: Third generation CALPHAD databases for 0K by automated statistical regression analysis.

ICAMS

Department Micromechanical and Macroscopic Modelling

MMM

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6. Department Micromechanical and Macroscopic Modelling

Prof. Dr. Alexander Hartmaier

▸ Research

Developing innovative materials that 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 derive such microstructure-property-relationships to predict macroscopic mechanical properties of materials, like strength, hardness, and fracture 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 laboratory experiment and introduce information about mechanisms or material parameters that have been derived from more fundamental scales, see *Figure 6.1* for an example about scalebridging in fracture modelling.

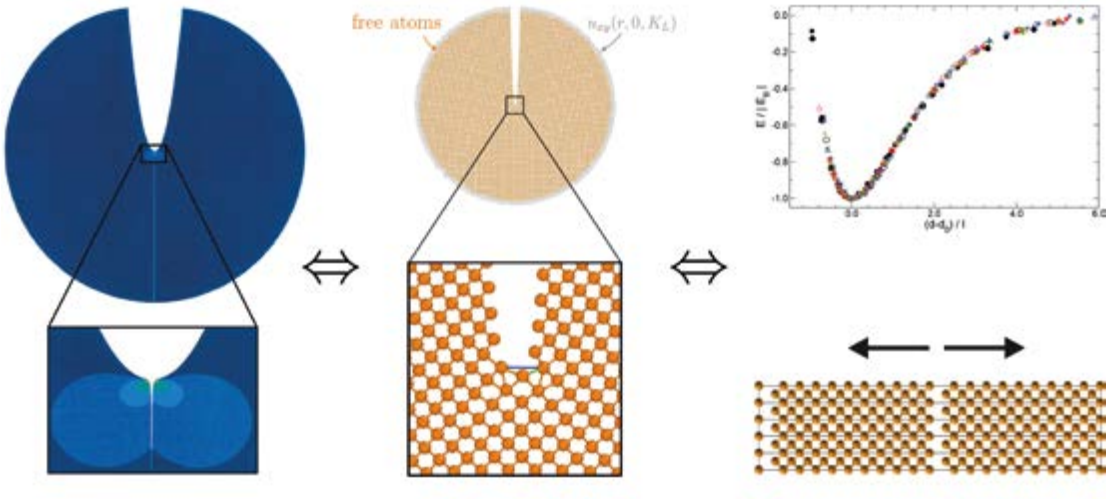

Fig. 6.1: A novel approach to bridge the scales from atoms to continuum in fracture modelling has been developed. With a physically consistent scaling law, data from density-functional calculations of atomic bond characteristics (right subfigure) can be directly applied in continuum fracture models (left subfigure). The approach has been validated with molecular dynamics simulations (middle subfigure), see Möller et al., JMR 33 (2018) 3750; https://doi.org/10.1557/jmr.2018.384.

Macromodels typically do not consider the microstructure of a material explicitly, but are based on the idea of homogeneous material behaviour, which is a severe restriction of such models. However, they can be very useful to identify critical regions with high mechanical stresses and strains within a component or loading conditions that are potentially damaging. At such critical spots, a micromechanical model is employed that explicitly takes into account the local microstructure and mechanical conditions, taken from the macro simulation and applied as boundary conditions to the microstructure model. The microstructure in such micromechanical models is described by representative volume elements (RVE) that 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. Such micromechanical models serve mainly two purposes: Firstly, they yield 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. Secondly, they provide the basis for macroscopic descriptions of material 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 homogenisation and can be used to take microstructural properties and mechanisms implicitly into account in macroscopic models of engineering problems. *Figure 6.2* shows an example of a micromechanical model of a polycrystal that couples crystal plasticity and diffusion of hydrogen through the microstructure. Elastic strains change the driving force for hydrogen diffusion and segregation, which is quantified by ab-initio density functional theory calculations. Furthermore, plastic strains alter the density of hydrogen trapping sites. Thus, such a coupling of mechanics and diffusion is important to understand the nature of hydrogen distribution within a microstructure, which is an essential mechanism of hydrogen embrittlement.

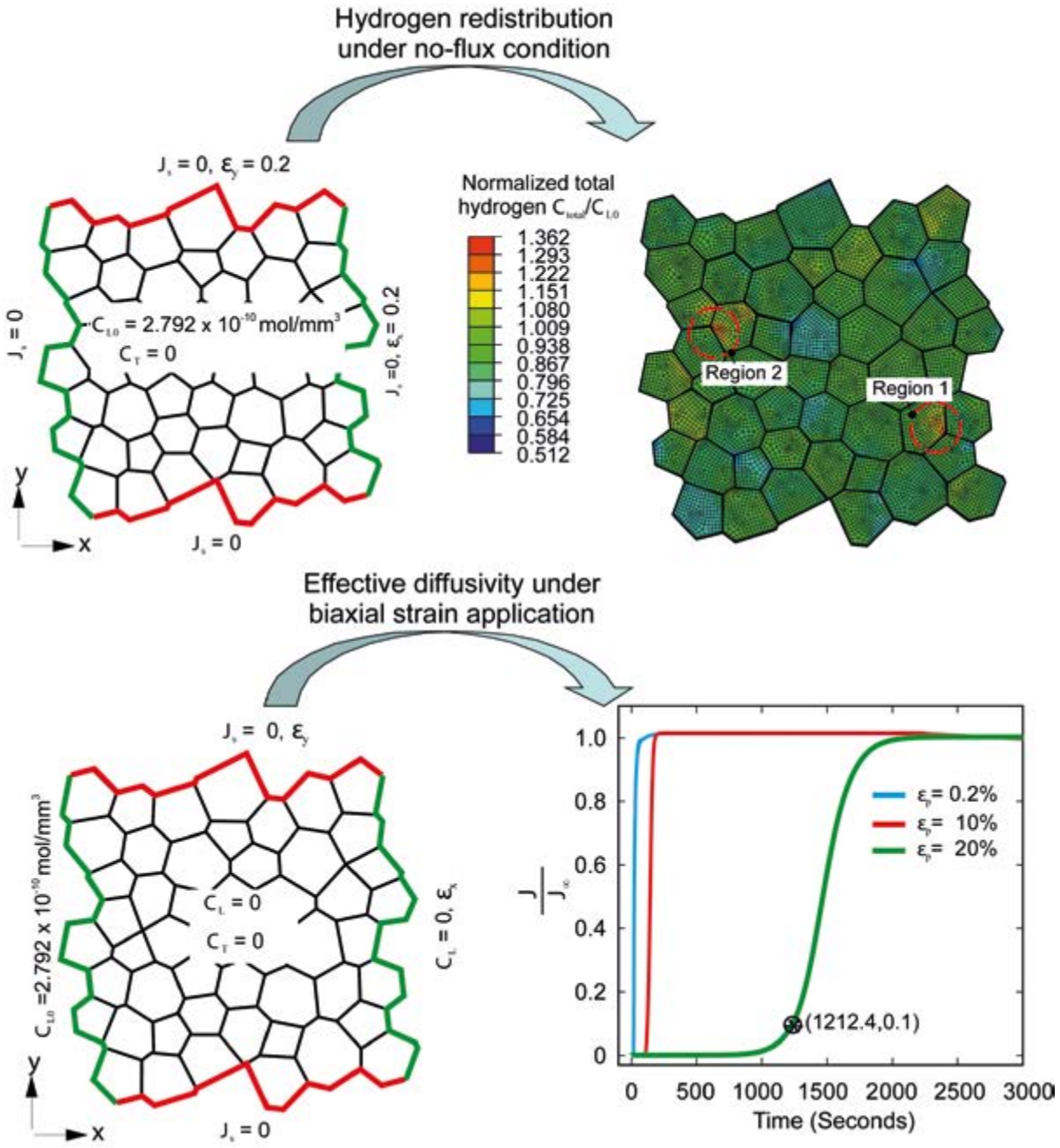

Fig. 6.2: Hydrogen diffusion through a microstructure is significantly affected by local elastic and plastic strains. Hence, a direct coupling of mechanics and diffusion kinetics is important to reveal the mechanisms of hydrogen redistribution in microstructures and how it contributes to hydrogen embrittlement. The top subfigure shows the results of the hydrogen redistribution within a predeformed microstructure, whereas the bottom subfigure demonstrates that this kind of modelling can be used to predict transient states of hydrogen diffusion kinetics that can be compared to experimental data, see ul Hassan et al. Phil. Mag. 99 (2019) 92, https://doi.org/10.1080/14786435.2018.1530466.

One increasingly important aspect of research in the department Micromechanical and Macroscopic Modelling is to establish links between numerical modelling and experiment. As seen in *Figure 6.3*, our models yield results that can be directly compared to experiment, which enables (i) their direct experimental validation, and (ii) the parameterisation of micromechanical models by inverse fitting to experimental data. In view of the relatively large number of model parameters, the latter approach is currently a major thrust direction of our research.

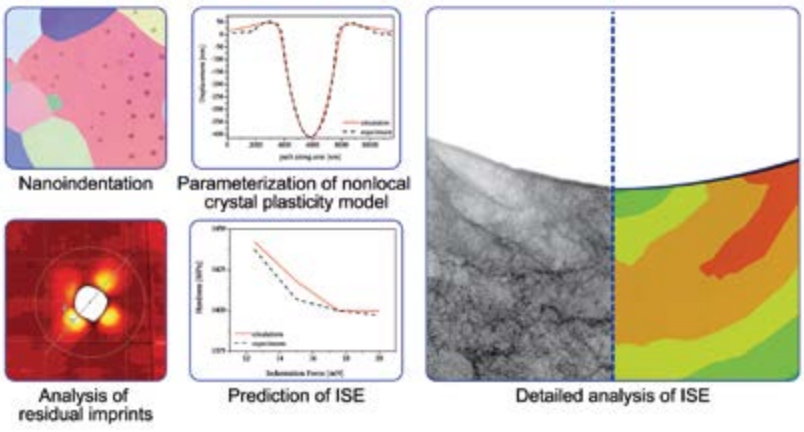

Fig. 6.3: Parameterisation of a non-local crystal plasticity model by inverse modelling of nanoindentation experiments supports our understanding of indentation size effects (ISE). Spherical nanoindentations have been performed in a coarse grained ARMCO iron polycrystal (top left) and the pile-up structures of individual imprints have been analysed (top middle). The parameters of a non-local crystal plasticity model have been adapted in an inverse procedure to yield the optimum comparability of the imprint topology between numerical simulation and experiment (bottom left). The thus-parameterised crystal plasticity model can predict the ISE found in experiment in a quantitatively correct way (bottom middle). A comparison of predicted and measured dislocation structures beneath the indentation supports our understanding of the mechanisms of this ISE, see Engels et al. Materialia 3 (2018) 21, https://doi.org/10.1016/j.mtla.2018.09.032.

As described above, predicting material 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 characterisation of realistic microstructures and local material properties has been one vital focus of the 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 that take into account dislocation density evolutions are combined with the phase-field code OpenPhase developed in the department STKS.

MMM

6.1. Mechanical Properties of Interfaces

Group leader:
Dr. habil. Rebecca Janisch

Group members:
Abril Azócar Guzmán
Ashish Chauniyal
Dr. Anupam Neogi

▸ Research

The research group Mechanical Properties of Interfaces carries out atomistic simulations to understand the fundamental processes occurring at interfaces under different loading conditions, which determine strength and deformability of polycrystalline microstructures in metals and alloys.

Ab initio electronic structure calculations based on density functional theory (DFT) are used to predict the energy, strength, and effective modulus of interfaces and other defects. These characteristic properties are used to derive and understand trends, give guidelines for alloy design and to establish constitutive relationships for multiscale simulations. Large scale molecular dynamics simulations are carried out to determine the fundamental deformation mechanisms – interfacial sliding and/or migration, dislocation emission, twinning – at different interfaces and temperatures during tensile and shear load, or during nano-indentation. If possible, these mechanisms are then related to fundamental physical quantities, such as bond length and energy, coordination numbers, and stacking fault energies.

In 2017/2018 the projects of the work group focused on the interplay between mechanical deformation and solubility and segregation in Fe alloys, including H embrittlement, on size effects in lamellar TiAl and the stability of different phases in TiAl alloys. Methodological work included the implementation of a design of experiment scheme to sample the energy space of grain boundaries, and the development of a force based scaling model that enables the use of DFT data in finite element simulations of fracture.

▸ Competences

- Ab initio electronic structure calculations
- Molecular dynamics simulations
- Scale-bridging modelling of interface mechanics and thermodynamics

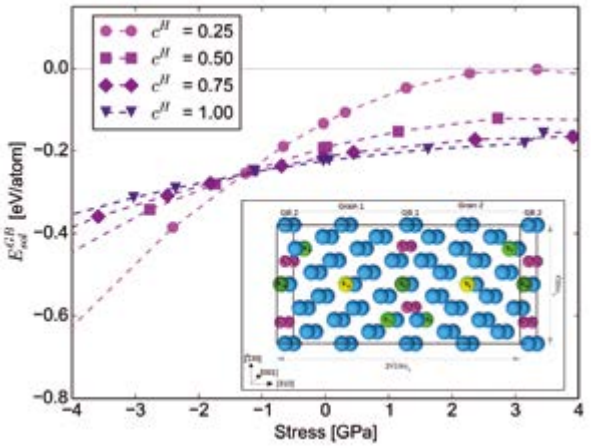

Fig. 6.4: Influence of tensile and compressive stress on the solution energy of hydrogen for different site occupancies at a Σ5 grain boundary in an Fe-C alloy. For compressive (tensile) stress, the lowest energies are obtained for minimum (maximum) concentration of H.

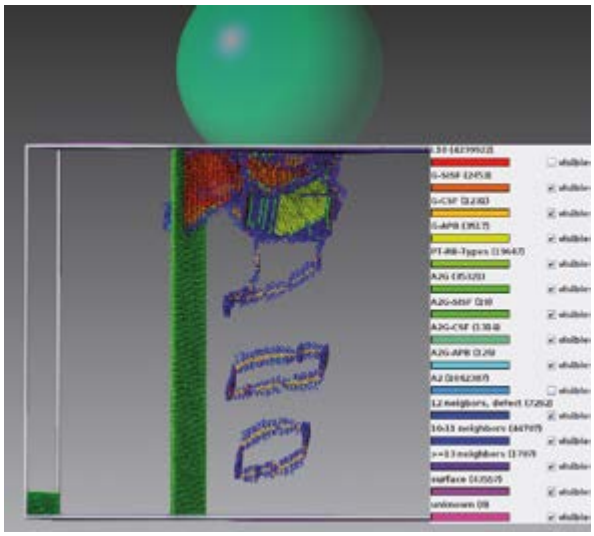

Fig. 6.5: Snapshot of a molecular dynamics simulation of nano-indentation into a two-phase Ti-Al alloy. Atoms with perfect coordination ($\alpha_2/L1_0$) are not shown. The interface between the two phases (layer of green atoms) confines the dislocation motion.

MMM

6.2. Micromechanics of Large Deformations

Group leader:
Dr.-Ing. Napat Vajragupta

Group members:
Waseem Amin
Abhishek Biswas
Jenni Kristin Engels
Dr.-Ing. Siwen Gao
Mahesh R. G. Prasad
Guru Prasad

▸ Research

The research group Micromechanics of Large Deformations aims at using the micromechanical modelling approach to describe large deformations of materials or components at the macroscopic scale. To achieve this goal, we focus on three research areas including: microstructure digitalisation; crystal plasticity models and parameterisation technique; and in-depth analysis of microstructure deformation.

Firstly, the method for digitalising microstructure is of crucial importance, because it must be able to capture important microstructural features such as: Grain size and shape distribution, texture, misorientation distribution etc. Hence, various platforms to generate microstructure models have been explored within our group. Our aim is to provide an industrial solution to digitalise microstructure, which are available for existing materials or microstructure design.

As new materials with more complex microstructures are constantly being developed, more advanced models are hence required to describe complex deformation mechanisms. Thus, we continuously intensify our expertise in crystal plasticity to consider multi-deformation mechanisms such as slip, phase transformations, and diffusional creep. In addition, inverse methods to parameterise material models are also within the scope of our work.

The combination of digitalised microstructure and material modelling allows us to investigate the dependence of deformation mechanisms on microstructural features. Based on the microstructure simulations, we predict macroscopic properties using homogenisation techniques, study the texture evolution during deformation, and change in other microstructural features.

▸ Competences

- Microstructure digitalisation
- Microstructure characterisation and analysis
- Crystal plasticity model
- Parameterisation of material models using inverse methods
- In-depth analysis of microstructure deformation

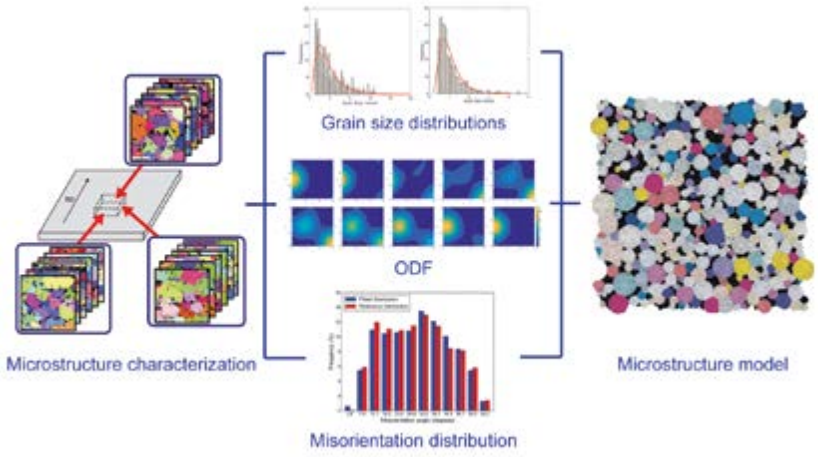

Fig. 6.6: Digitalisation of a microstructure. The process starts from microstructure characterisation using EBSD. Results are then quantitatively characterised to obtain grain size distribution of each constituents, Orientation Distribution Function (ODF), and misorientation distribution. The method currently under development aims to generate microstructure models, which quantitatively mimic these microstructural features.

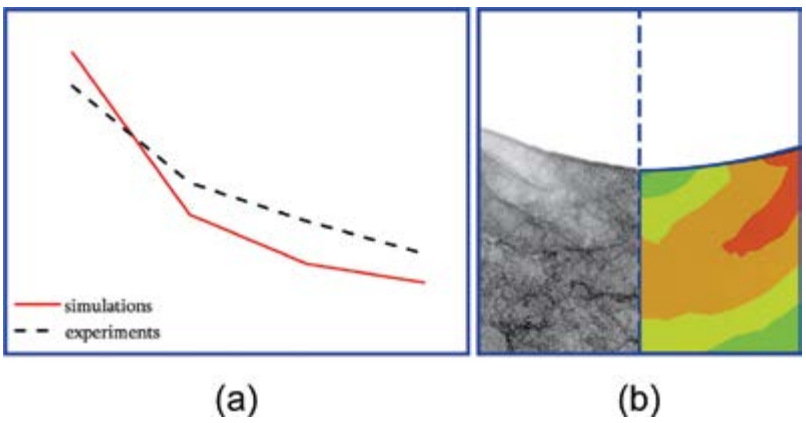

Fig. 6.7: Analysis of the Indentation Size Effect (ISE) in spherical nanoindentation by experiment and non-local crystal plasticity. In this work, ISE can be observed in the parameterised nanoindentation models which are also in a good agreement with experimental results (a). By analysing residual imprints from both experiments and simulations, one can better understand the mutual contributions of geometrically necessary dislocations (GND) and statistically stored dislocations (SSD) to the material response (b).

MMM

6.3. Discrete Micromechanics and Fracture

Group leader:
Dr.-Ing. Hamad ul Hassan

Group members:
Dr. Masud Alam
Denise Reimann
Hafiz Muhammad Sajjad
Ibrar Saleh
Zhanfeng Wang

▸ Research

The Discrete Micromechanics and Fracture group carries out multi-disciplinary research regarding the response of advanced engineering materials 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. Experiments are performed to generate reliable input data and to validate the virtual experiments in collaboration with other groups.

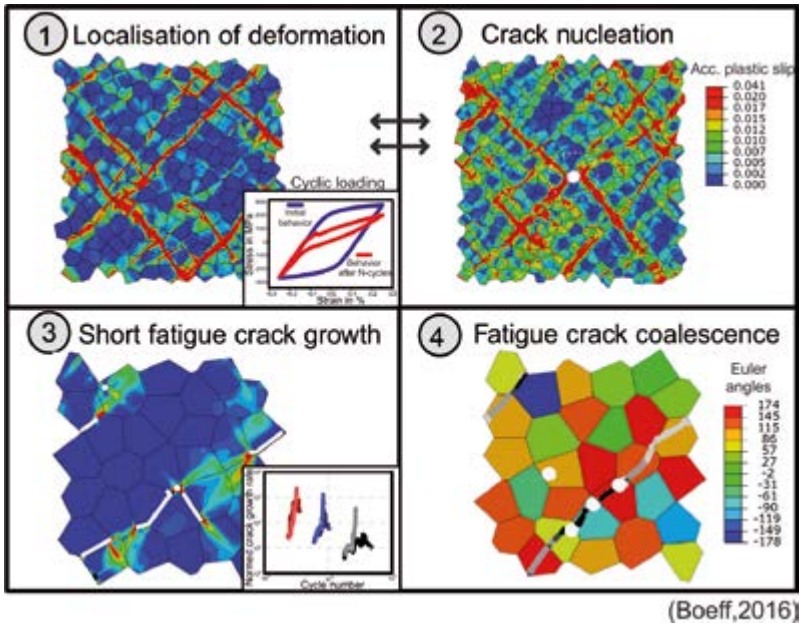

Fig. 6.8: Numerical simulation of fatigue behaviour using the Crystal Plasticity-Finite element method (CP-FEM). (1) Localisation of deformation under cyclic loading (2) Crack nucleation due to accumulation of plastic slip (3) Short fatigue cracks grow individually (4) Coalescence of several cracks through multiple grains.

Our analysis of localised 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 and the components made from them. A major emphasis of this group is to understand how the internal microstructure of an engineering material influences its response during application in the field. Investigations are carried out based on micromechanical principles using Crystal Plasticity-Finite element method (CP-FEM) to describe their plasticity, fracture, damage, and fatigue behaviour. The influence of hydrogen environment on the fracture behaviour of the materials is also investigated. Another important application area is the numerical modelling of nano/micro-machining. 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 on modelling of microstructures and the atomistic description of fracture.

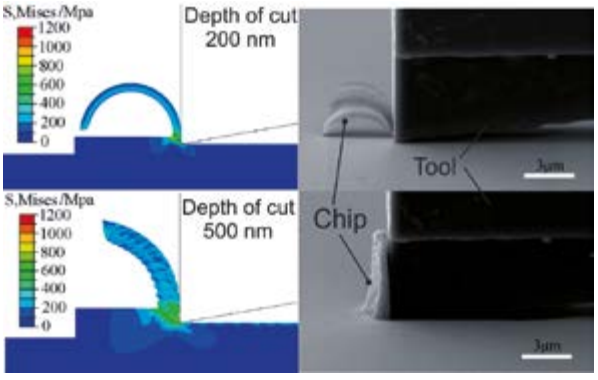

Fig. 6.9: Comparison of micro-cutting simulations with experiments for different depths of cut.

▸ Competences

- Micromechanical material characterisation
- Damage and fatigue analysis
- Numerical modelling of machining
- Micromechanical simulation of fracture
- Cohesive zone modelling and hydrogen embrittlement

ICAMS

High-Performance Computing in Materials Science

HPC

7. High-Performance Computing Materials Science

Prof. Dr. Godehard Sutmann

Group members:
Dr. Carlos Teijeiro
Dr.-Ing. Marvin Tegeler
Dr.-Ing. Hariprasath Ganesan
Stephan Schulz

▸ Research

The research group 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 original research, the group is linked to the other ICAMS departments and supports the development of simulation codes and efficient parallelisation of programs, developed at ICAMS. Currently, a focus is given to new approaches for continuum modelling for plastic deformation and efficient ways to balance the computational work on large parallel clusters. These works are linked to the ICAMS departments "Scalebridging Thermodynamic and Kinetic Simulation" (STKS) and "Micromechanical and Macroscopic Modelling"(MMM). Key elements in these groups are in-house developed codes, e.g. OpenPhase, which have the potential to develop as community codes and which are applied for a variety of problems at ICAMS. Research and development is performed in close cooperation with the Jülich Supercomputing Centre at Forschungszentrum Jülich.

For the continuum description of materials properties an Euler-Lagrangian method is further developed, which is based on the materials point method. It is especially useful for problems involving the dynamics of history dependant materials and large deformations. The advantage of particle based simulation methods in plastic deformation is the independence of a mesh and therefore, remeshing can be avoided. However, there are challenges like time stepping, energy conservation or treatment of boundary conditions, which are considered to make the method accurate and efficient. A code has been developed which is parallelised using orthogonal domain decomposition. Two different methods of communication have been considered based on MPI or coarrays as introduced in Fortran 2008. The possible materials are implemented from their constitutive equations and most models can be easily added to the code. Currently, the simple Hooke's Law is supported as well as a hyper-elastic Neo-Hookean model. For testing purposes a few non-solid models are also implemented such as a model for a simple inviscid fluid and a Drucker-Prager based model for sand.

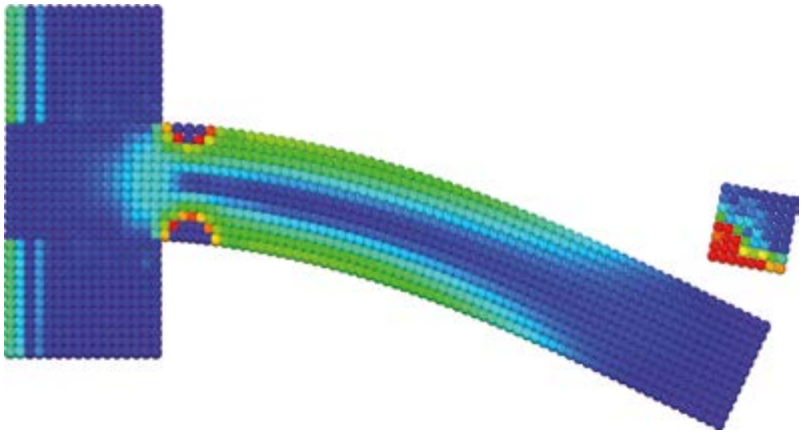

Fig. 7.1: Stress field distribution of an elastic bar and brick, colliding with each other, computed with the Euler-Lagrange MPM method.

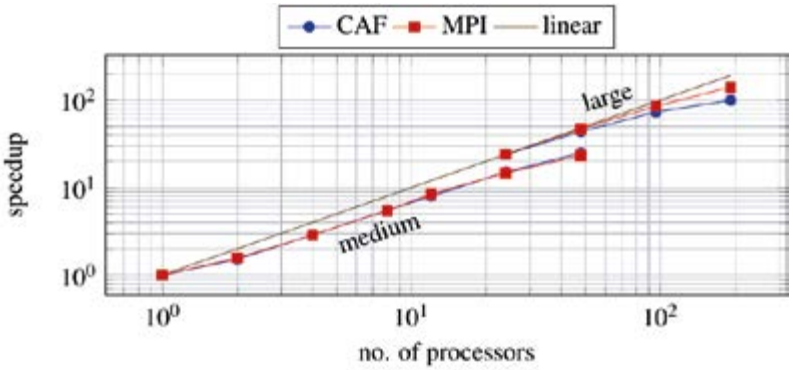

Fig. 7.2: Scaling behaviour of the MPM method as implemented by the Co-Array Fortran and the MPI communication protocols.

Based on the phase-field method, a procedure has been developed which allows to construct microstructure models, which reproduce experimentally observed grain size distributions. For micro-mechanical modelling it is important to use representative structures for materials, as they are observed in experiments. One essential feature is the distribution of grain sizes, for which distribution functions are sometimes available. In the present approach, a certain number, N, of seed particles is placed inside a box of fixed size. Then a nucleation process is simulated by the phase-field method for N nuclei. The growing of the individual phase is then controlled by the driving force, which is adjusted to be proportional to the grain size, corresponding to the statistical distribution of the grain sizes. In this respect, the model is physically motivated, leading to a structure with surface tension equilibrium between the different phases.

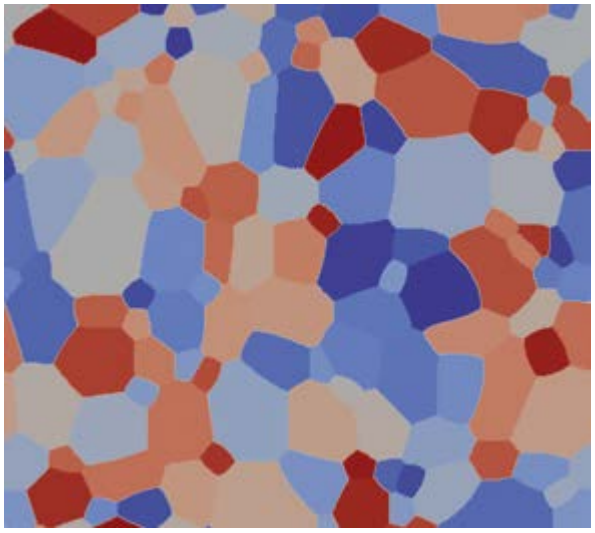

Fig. 7.3: Microstructure obtained with the phase-field method, following results obtained experimentally for grain size distributions.

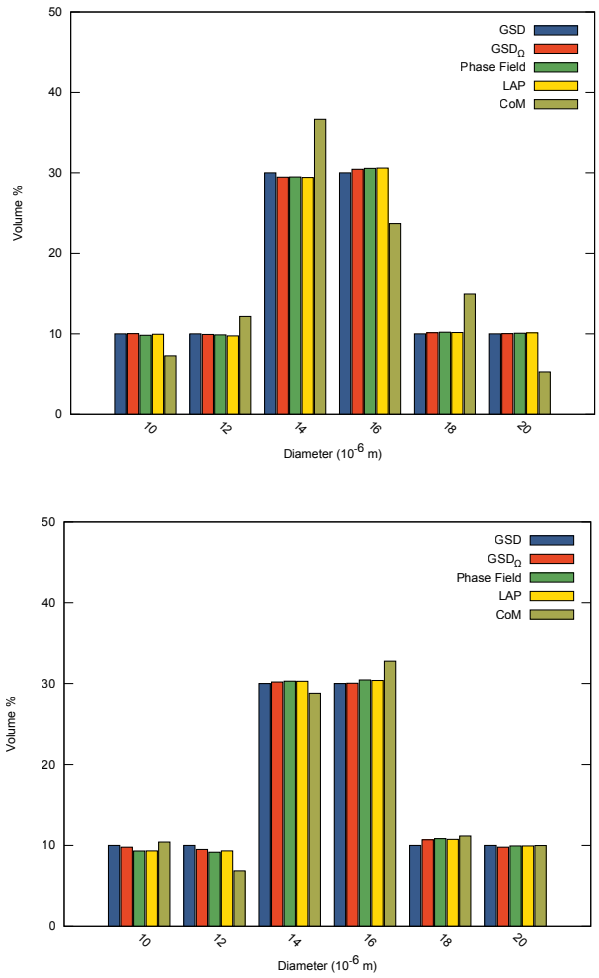

Fig. 7.4: Comparison of distribution functions of grains with indicated size in 2d (above) and 3d (below) computations with pure phase-field method and CoM or LAP reconstruction.

Segregation phenomena have been studied with a newly developed hybrid Molecular Dynamics/ Monte Carlo method. The very slow driven diffusion process which is underlying segregation of interstitial atoms towards lattice defects has been considered via stochastic trial moves, followed by MD relaxation processes. For T=0K conditions, this corresponds to stochastic optimisation, which has been improved by a biased Monte Carlo sampling procedure. Extensions to T>0K have been considered by a mean field approach, which is justified for moderate temperatures. The technique has been tested for single dislocations as well as dislocation networks, produced in nano-indentation experiments. The method has been parallelised with both simple manager/worker approaches, which are suitable for small number of processors, as well as with a domain decomposition approach, which implements a multi-manager technique, reducing strongly the administration overhead of a single manager. With this technique, larger number of processors could efficiently be used, which makes it possible to simulate also multi-million atom systems.

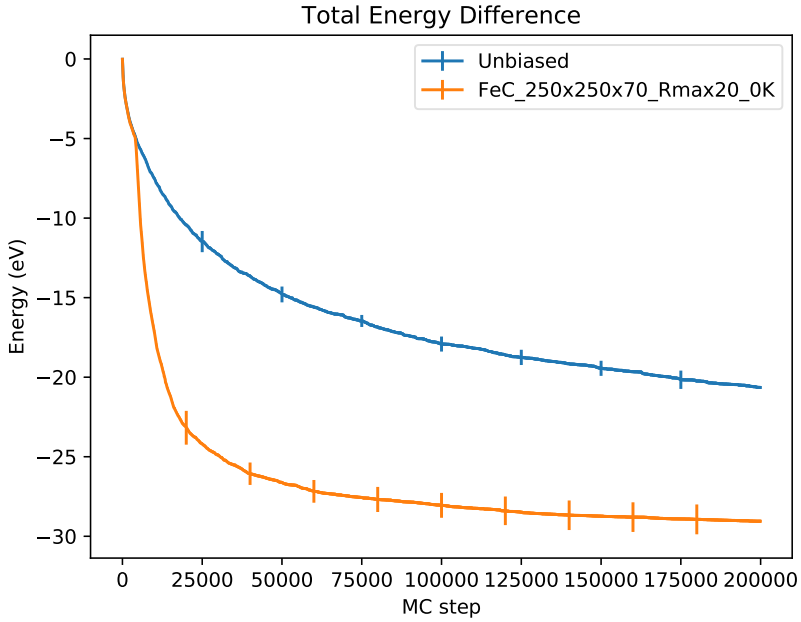

Fig. 7.5: Comparison of system configuration energies of the unbiased and biased Monte Carlo approach, respectively.

ICAMS

Advanced Study Group Modelling

8. Advanced Study Group Modelling

Prof. Dr. Jörg Neugebauer
Dr. Tilmann Hickel

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, in particular on the electronic scale. It develops, implements, and applies ab initio guided computational methodologies and toolsets that allow for an accurate prediction of properties of advanced structural and functional materials in realistic environments.

Being mainly located in the department of Computational Materials Design at the Max-Planck-Institut für Eisenforschung in Düsseldorf, the complex atomic-based mechanisms in steels form a central part of the contribution to ICAMS. In the last years, the ASG developed, for example, computational tools to describe the sophisticated interplay of lattice and magnetic degrees of freedom and therewith structural transformations in Fe-based alloys at finite temperatures. At the same time, the chemical complexity and atomic structure of confined and extended defects in various metals is addressed with novel approaches. Hardening mechanisms such as the mechano-chemical coupling during precipitate formation, as well as degradation mechanisms such as hydrogen embrittlement are jointly investigated.

Since the underlying highly accurate and computationally efficient methods require complex simulation protocols, the ASG developed over the last years pyiron – a platform that provides an integrated development environment to implement, test and employ computational tools. It does not only provide the user with a standardised interface for the communication between different codes and routines, but also allows easy upscaling to high-throughput studies. As a result, the time needed to become acquainted with new tools is dramatically reduced, productivity is boosted and the exchange with external partners and particularly with ICAMS is supported.

Fig. 8.1: The ADIS2018 (Ab initio Description of Iron and Steel) workshop in Ringberg was the seventh workshop of a biennial series that is jointly organized by the ASG Modelling and the AMS department.

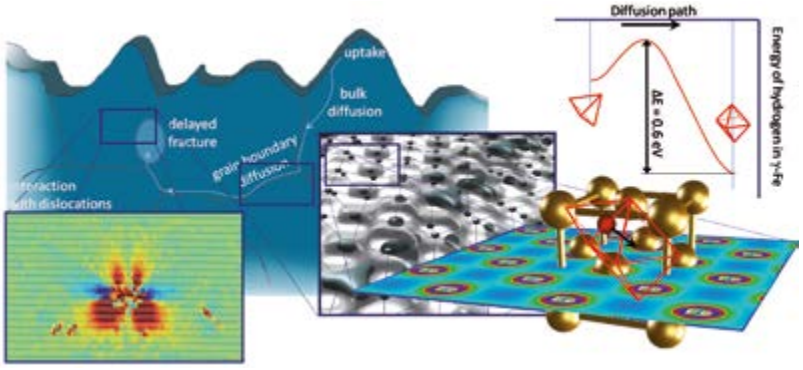

Fig. 8.2: The ASG Modelling addresses a variety of processes related to hydrogen embrittlement. This includes ab initio studies on the solution/diffusion of hydrogen in bulk phases/grain boundaries, kinetic Monte-Carlo simulations based on ab initio diffusion barriers and the investigation of atomistic mechanisms such as hydrogen enhanced local plasticity.

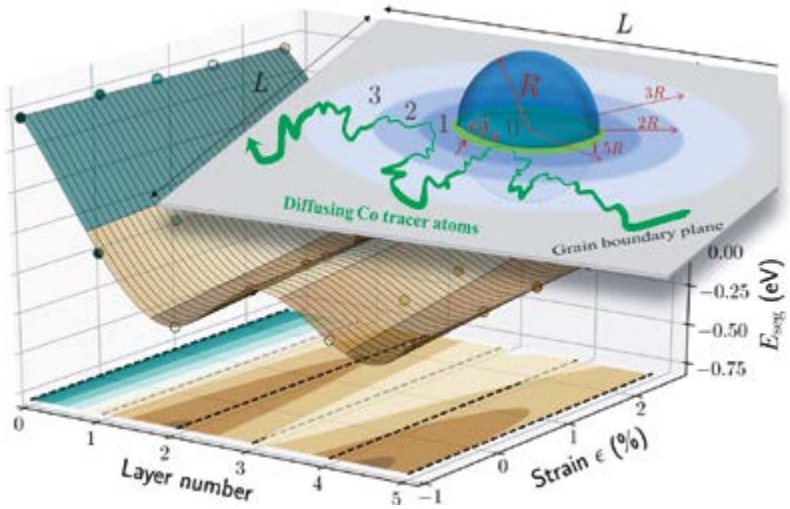

Fig. 8.3: Schematic illustration of the employed diffusion model for tracer particles (inset) together with the particle segregation energy surface in the misfit strain field of a Al_3Sc nanoprecipitate.

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Advanced Study Group Input Data and Validation

9. Advanced Study Group Input Data and Validation

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

The Advanced Study Group "Input Data and Validation" is active in a broad range of research fields. In this report we present two important research examples. In the first one, we consider high temperature shape memory alloys (HTSMAs). Research on HTSMAs has been performed in the frame of the DFG research unit FOR 1766 where scientists from different universities (Hannover, Bochum, Kassel and Munich) collaborate. The shape memory effect allows a material to re-establish its prior geometry after a strong deformation which significantly exceeds conventional elastic strains. The effect relies 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. *Figure 9.1* exemplarily shows the microstructure of a Ti-Ta HTSMA where martensitic structures can be seen.

Recently, we have studied new Ti-Ta-based HTSMA compositions which provide a significantly improved functional performance. In contrast to other HTSMAs, e.g. Ni-Ti-based alloys, our Ti-Ta-based HTSMAs provide sufficient ductility such that semi-parts like bars, rods, sheets and wires can be easily prepared by conventional processing techniques. *Figure 9.2* exemplarily documents the functional behaviour of a Ti-Ta-based HTSMA spring actuator which has been prepared by our research group. The spring is mounted in a test rig where it is loaded with a weight. During direct current heating, the actuator transforms back into the high temperature phase. In parallel, the spring contradicts, trying to re-establish its prior geometry. Recently, new Ti-Ta compositions were identified by Alberto Ferrari, Jutta Rogal and Ralf Drautz using DFT calculations. We were able to validate their predictions and to demonstrate that these materials exhibit a significantly improved functional stability.

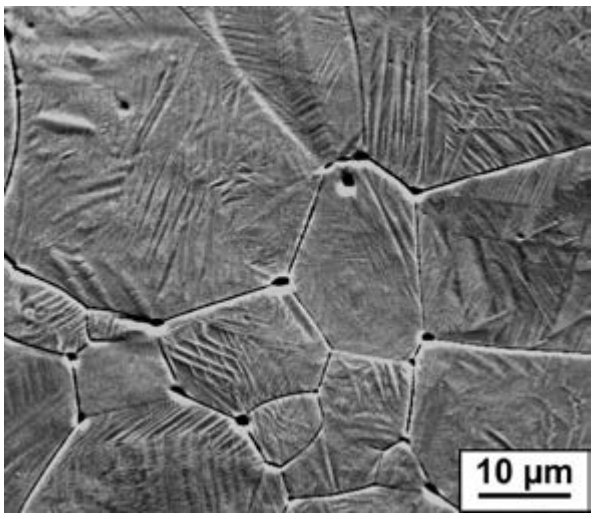

Fig. 9.1: Martensite in a Ti-Ta high temperature shape memory alloy (scanning electron microscopy image).

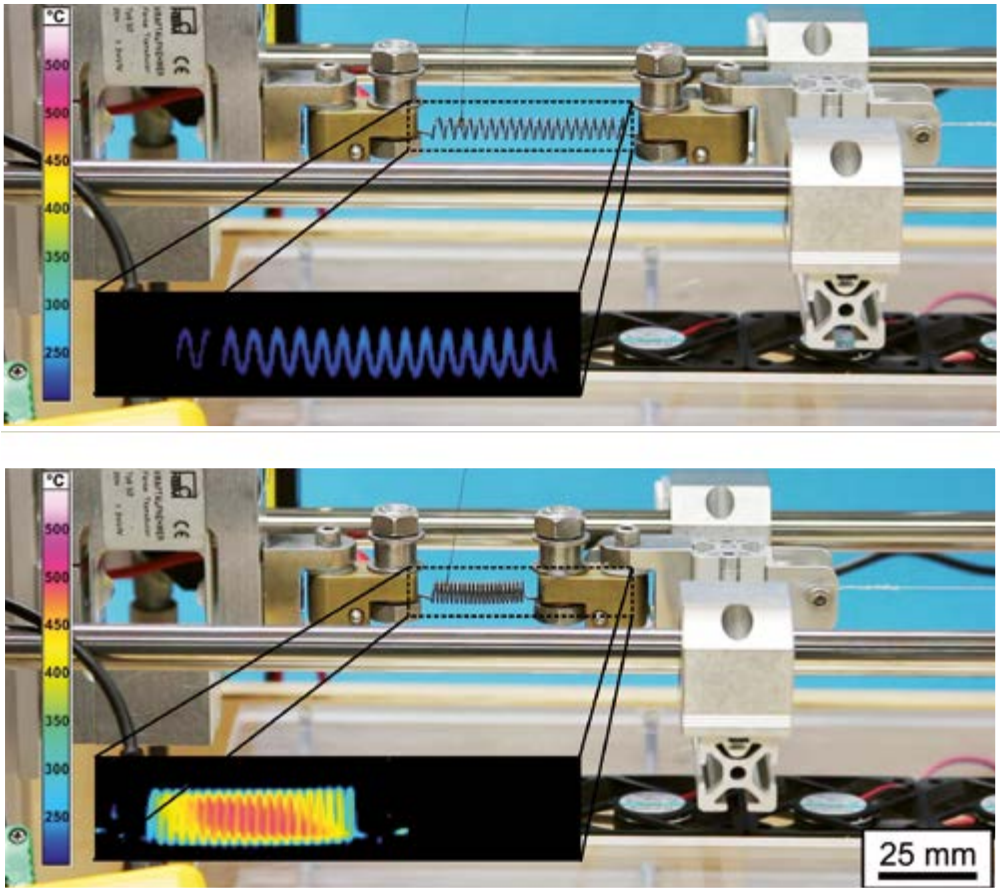

Fig. 9.2: Thermally induced shape memory effect in a Ti-Ta-based high temperature shape memory spring actuator during direct current heating. Temperature distributions in the spring are monitored by infrared thermography (see insets).

As a second research example we now consider nickel base superalloys. Superalloys represent key materials for modern gas turbines which operate in electric power plants and in aero engines. They withstand high mechanical loads at high temperatures (e.g. 1000°C) and they allow for high efficiencies and thus reduced emission of greenhouse gases. Our research activities on superalloys are conducted in the frame of the collaborative research centre SFB/Transregio 103 (Superalloy Single Crystals – From Atoms to Turbine Blades), which is in its second funding phase. In project B7 of SFB/Transregio 103 we investigate the formation of crystal defects, such as low angle grain boundaries and dislocations, which often form during dendritic solidification of superalloy melts. We investigate how important solidification parameters affect the formation of these defects. The nature of this research made it necessary to develop new / improved characterisation techniques. We recently developed a new electron back scatter diffraction (EBSD) procedure which provides a significantly higher angular resolution as conventional EBSD. Our rotation vector base line (RVB-)EBSD uses cross-correlation analysis in combination with a multi-dimensional corrective base-line function for the interpretation of diffraction data. This new technique allows to study smallest crystallographic orientation changes in Ni-base superalloys. *Figure 9.3* presents new microstructural results from an as-cast superalloy. Two dendrites are shown which grow parallel to the viewing direction. The two images present information on local alloy chemistry *(Figure 9.3a)* and on local crystallographic orientation *(Figure 9.3b)* of the same microstructural region (see reference point "P" in both images). The RVB-EBSD data rely on a colour-code which is specified in the pole figure. Our RVB-EBSD technique reveals changes in crystal orientation which are significantly smaller than 0.05°. As a striking result, the color-coded crystal orientation map in *Figure 9.3b* clearly shows dendritic features. This finding suggests that local changes in alloy chemistry during dendritic solidification *(Figure 9.3a)* result in specific changes in local crystallographic orientation. We will use this new EBSD technique to study the effects of different solidification conditions in the near future.

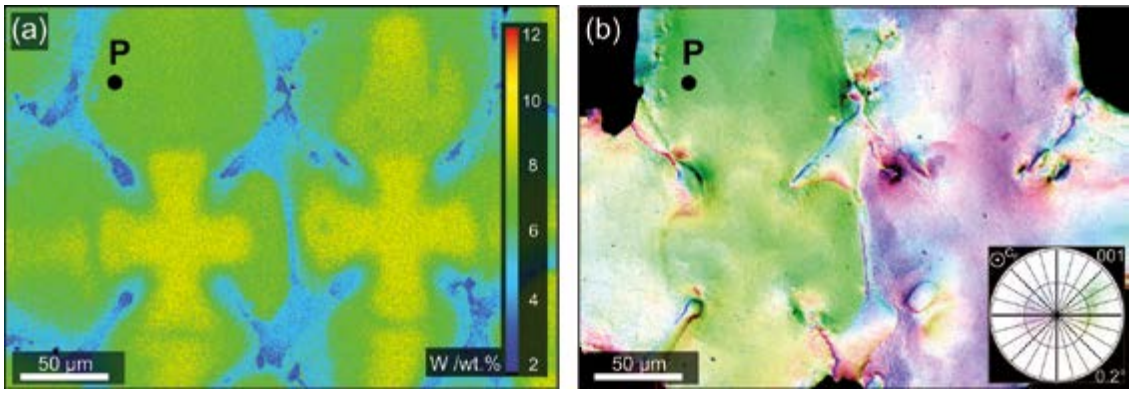

Fig. 9.3: New microstructural results on dendritic microstructures in single crystal nickel-base superalloys. (a) Chemical composition mapping of the element tungsten, obtained by electron probe micro analysis (EPMA). (b) New crystal orientation mapping of the same region as shown in Figure 9.3a using our new rotation vector base line EBSD technique. Crystal orientation changes below 0.2° are presented.

IC∧MS

Advanced Study Group Processing and Characterisation

10. Advanced Study Group Processing and Characterisation

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

The research activities of the ASG Processing and Characterisation located at the Institut für Eisenhüttenkunde (IEHK) at RWTH Aachen involve the major topics materials characterisation, advanced computer simulation of materials, materials processing, and damage mechanics. The ultimate aim is to understand the mechanisms behind the physical, mechanical, and microstructural properties of steels and other advanced engineering alloys, 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 metals and alloys at sub-zero temperatures as well as room and elevated temperatures.

Using a suitable combination of microstructural design, process optimisation, 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.

Recently, the ASG Processing and Characterization has been involved in several projects focussing on the Integrative Computational Materials Engineering (ICME). These projects focussed on the idea to identify required mechanical property profiles for improved component performance via macroscopic damage mechanics modelling, to translate these requirements into optimised microstructural configurations, and to find the corresponding parameters of thermo-mechanical treatments that would allow to precisely adjust these desired microstructures. Several components and application fields were selected to demonstrate the efficiency of the new approach, ranging from pipelines for oil and gas transportation to automotive components relevant for crash safety. In the future, the simulation framework will be enriched in order to take influences of manufacturing (e.g. cold forming, turning, and welding) on the component behaviour into account. Furthermore, the simulation framework will be extended in the direction of additive manufacturing.

The ASG Processing and Characterisation contributes to TRR 188 "Damage Control in Forming Processes" via project B05 "Damage-tolerant material design". In this project, ductile damage in multi-phase steels is modelled on different scales which are connected by a weak coupling. The aim of the project is to increase the damage

tolerance by microstructure design and to identify the acceptable amount of forming-induced ductile damage for a pre-defined component performance. Since the relevant load case can be a cyclic one, the project also studies the interaction between ductile damage and fatigue mechanisms.

Furthermore, the ASG contributes to the priority program SPP 1713 "Strong coupling of thermo-chemical and thermo-mechanical states in applied materials" by the project M4 "Modelling bainitic transformations during press hardening". The main goal of the project is to develop a bottom-up understanding of bainitic transformations in particular under the influence of applied stresses, and to set the path for a theory-guided improvement of processing steps during advanced press hardening of high-strength steel sheet components for safety applications.

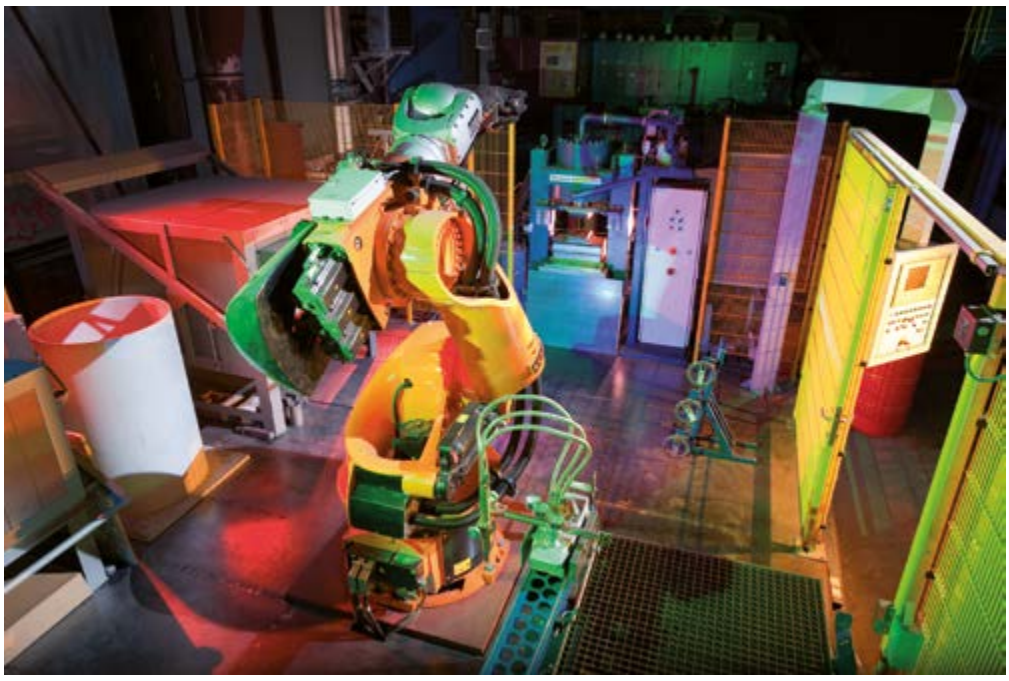

Fig. 10.1: SemiProductSimulationCenter at IEHK.

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Advanced Study Group Diffusion and Microstructure Analysis

11. Advanced Study Group Diffusion an Microstructure Analysis

Prof. Dr. 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 at 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 atomic transport, atomic-level structure and thermodynamic properties of different materials ranging from high-entropy alloys (HEAs) including Compositionally Complex Alloys (CCAs), ordered and partially ordered intermetallic phases, and bulk metallic glasses. The impact of plastic deformation on microstructure and property evolution in these materials is investigated on all scales.

In *Figure 11.1* the results of a detail analysis of the nano-beam diffraction patterns taken at different specific location of plastically deformed Zr-based bulk metallic glass are shown. The medium-range order of both as-cast and deformed states was characterised by variable resolution fluctuation electron microscopy. As a result of deformation, two distinct medium-range order cluster types are found to be formed in both matrix and shear bands.

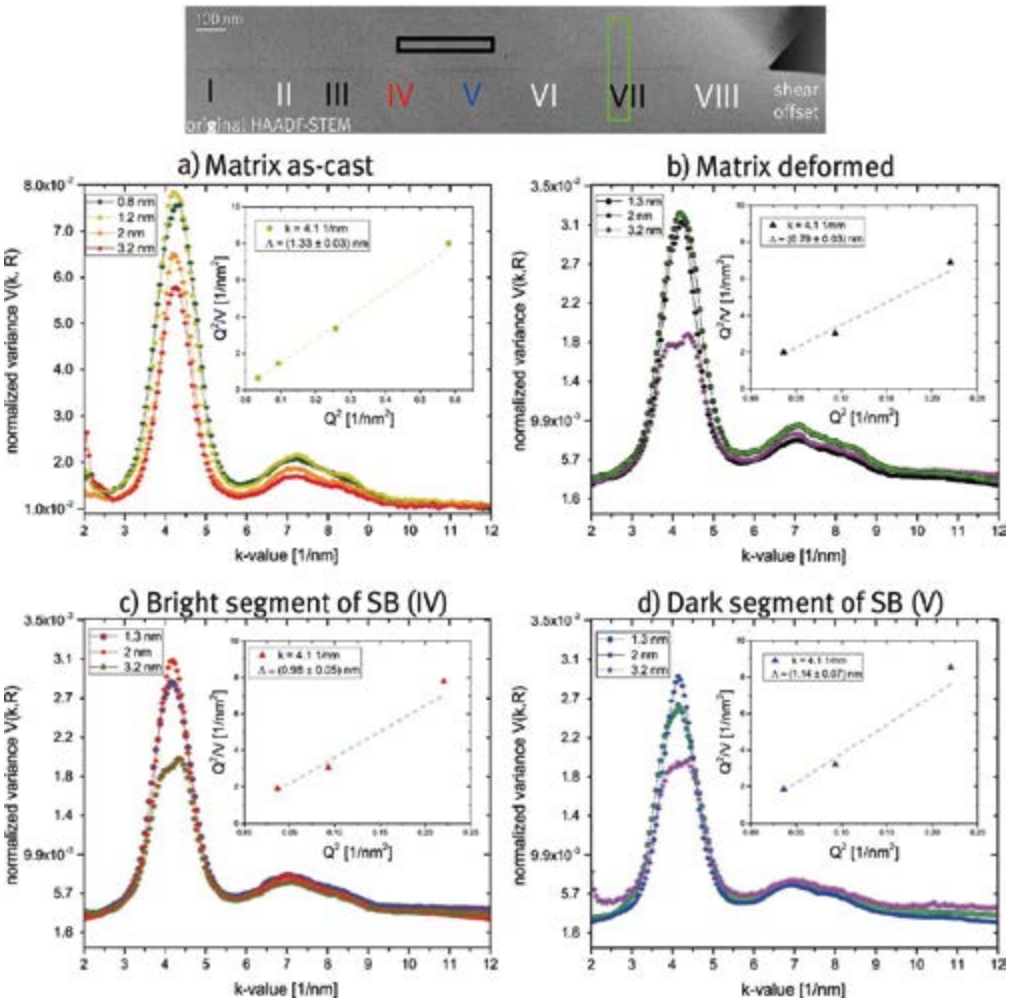


Fig. 11.1: Normalised variance profiles with variable probe sizes (0.8 nm, 1.3 nm, 2.0 nm and 3.2 nm) calculated from nano-beam diffraction patterns of (a) as-cast state of the matrix, (b) the matrix next to the shear band indicated by the black box in the TEM image, (c) the bright SB segment (IV) and (d) the dark SB segment (V) shown in TEM image. The insets in (a) - (d) show the pair-persistence analysis for the as-cast state, the matrix next to the shear band, bright (IV) and dark (V) shear band segment using reciprocal k-values of 4.1 nm^{-1}.

For the first time, bulk tracer diffusion coefficients of Co, Cr, Fe and Mn were determined in polycrystalline CoCrFeNi and CoCrFeMnNi HEAs using the radiotracer method. The homogeneity of the material was carefully analysed using atom probe tomography. The temperature dependencies of bulk diffusion for all tracers show Arrhenius behaviour. The corresponding activation energies (Q) and the logarithm of pre-exponential factors (D_0) show a linear relationship, thus following the "compensation rule" *(see Figure 11.2)*.

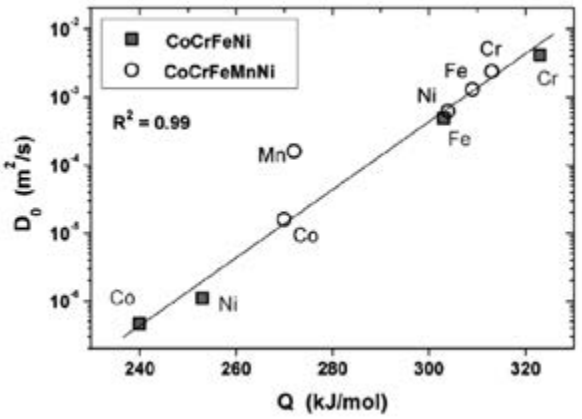


Fig. 11.2: The pre-exponential factors (D_0) for bulk diffusion of the constituent elements in CoCrFeNi (squares) and CoCrFeMnNi (circles) as a function of the corresponding activation energy Q. All elements except of Mn reveal an almost linear dependence (solid line).

The diffusion kinetics in a CoCrFeMnNi high-entropy alloy is investigated by a combined radiotracer-interdiffusion experiment applied to a pseudo-binary $Co_{15}Cr_{20}Fe_{20}Mn_{20}Ni_{25}$/ $Co_{25}Cr_{20}Fe_{20}Mn_{20}Ni_{15}$ couple, (see *Figure 11.3)*. As a result, the composition-dependent tracer diffusion coefficients of Co, Cr, Fe and Mn are determined. In order to ensure a consistent treatment of tracer and chemical diffusion a generalised symmetrised continuum approach for multi-component interdiffusion is proposed. Both, tracer and chemical diffusion concentration profiles are simulated and compared to the measurements. By using the measured tracer diffusion coefficients the chemical profiles can be described, almost perfectly, including up-hill diffusion, (see *Figure 11.4*). Note that the up-hill diffusion is not reproduced using the existing mobility databases.

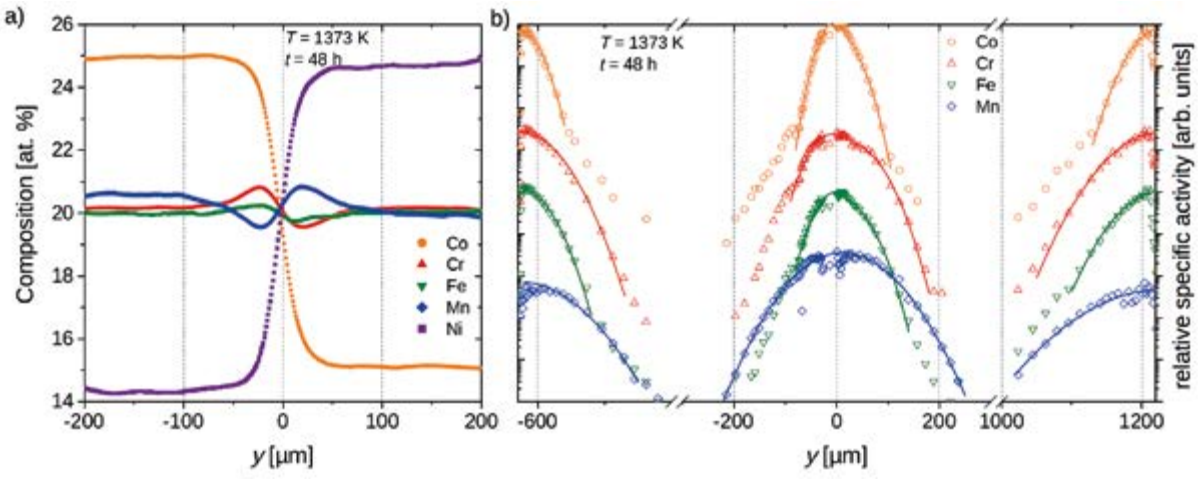


Fig. 11.3: a) EPMA-analysis of the constituents at the interface and b) penetration profiles measured for tracer ^{57}Co, ^{51}Cr, ^{59}Fe and ^{54}Mn diffusion (open symbols) from the outer surfaces and the internal source located at the original interface between the two alloys (the Gaussian fits are represented by the straight lines). In b) the tracer profiles are shifted by multiplication with a constant factor for a better readability.

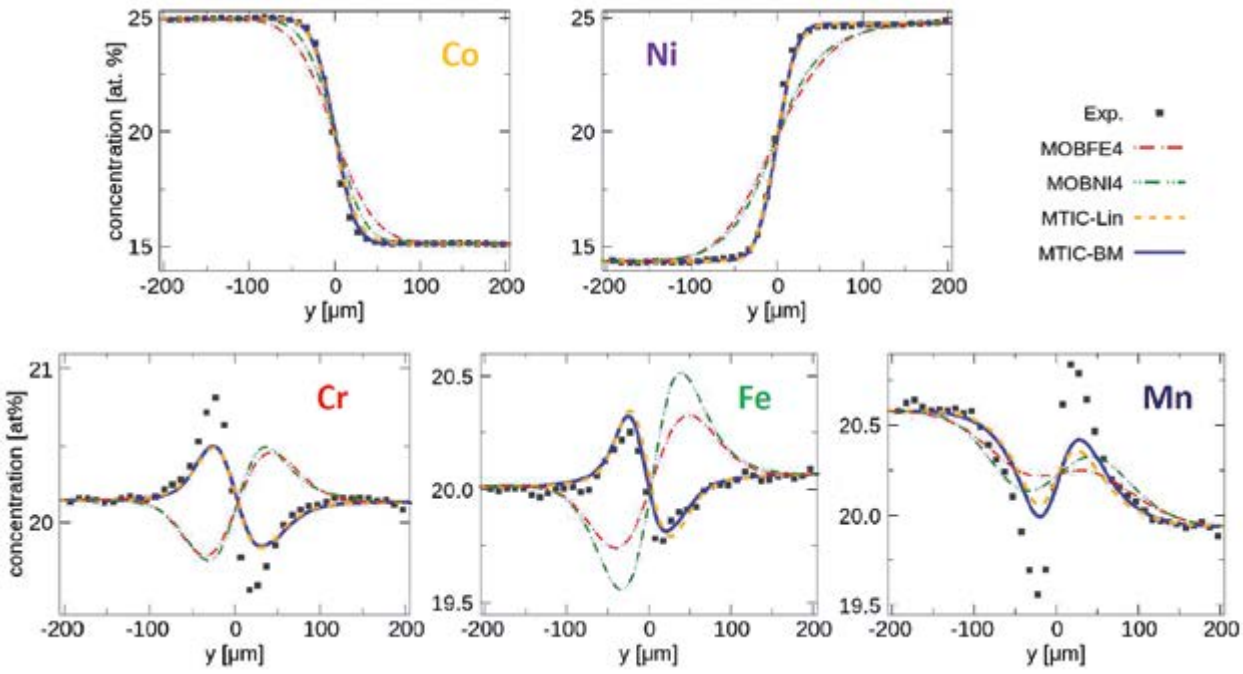


Fig. 11.4: Comparison between experimentally obtained interdiffusion profiles and simulated ones using the HEA-databases combined with different atomic mobility databases for all five elements (Co, Cr, Fe, Mn and Ni) after 48 h at 1373 K.

ICAMS

Research Highlights

12. Research Highlights

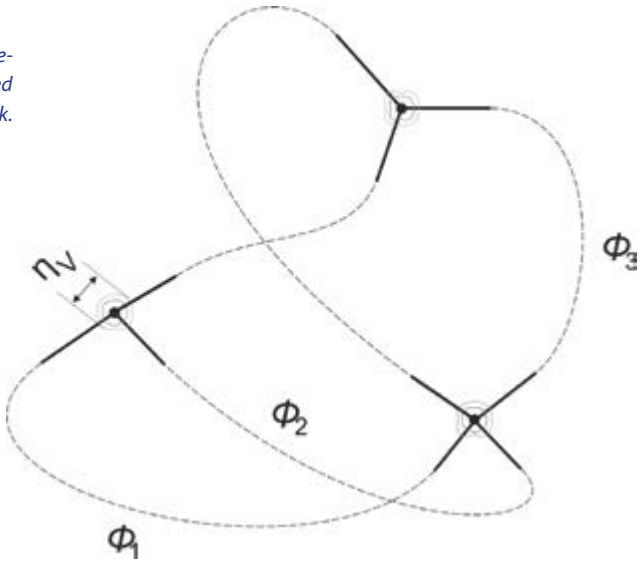
2017

Quantum-phase-field concept of matter: Emergent gravity in the dynamic universe

I. Steinbach

Zeitschrift fur Naturforschung A, **72**, 51-58 (2017)

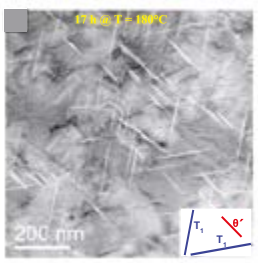
A monistic framework is set up where energy is the only fundamental substance. Different states of energy are ordered by a set of scalar fields. The dual elements of matter, mass and space, are described as volume- and gradient-energy contributions of the set of fields, respectively. Time and space are formulated as background-independent dynamic variables. The evolution equations of the body of the universe are derived from the first principles of thermodynamics. Gravitational interaction emerges from quantum fluctuations in finite space. Application to a large number of fields predicts scale separation in space and repulsive action of masses distant beyond a marginal distance. The predicted marginal distance is compared to the size of the voids in the observable universe.

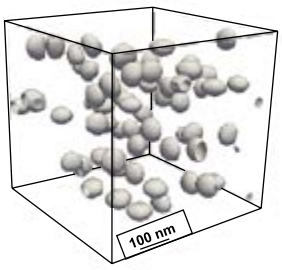


Scheme of a number of five quantum-phase-fields forming three elementary particles as junctions. The junctions and fields can be pictured as knots and ropes respectively, forming a multi-dimensional network.

Precipitation of T_1 and θ´ Phase in Al-4Cu-1Li-0.25Mn during age hardening: Microstructural investigation and phase-field simulation

I. Häusler, C. Schwarze, M. U. Bilal, D. Valencia Ramirez, W. Hetaba, R. Darvishi Kamachali, B. Skrotzki
Materials, **10**, 117 (2017)



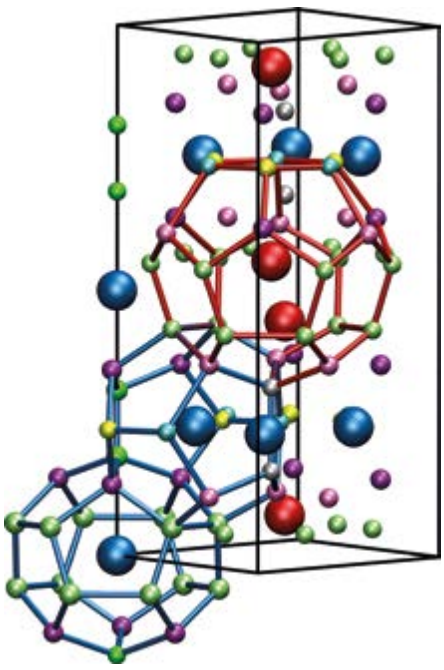


T_1 and θ´phases simultaneously form and evolve in Al-Cu-Li system. 3D phase-field simulation of θ´ precipitates qualitatively confirm distribution and size evolution of these precipitates during age hardening.

Experimental and phase-field studies of age hardening response of a high purity Al-4Cu-1Li-0.25Mn-alloy (mass %) during isothermal aging are conducted. In the experiments, two hardening phases are identified: the tetragonal θ´ (Al_2Cu) phase and the hexagonal T_1 (Al_2CuLi) phase. Both are plate shaped and of nm size. They are analyzed with respect to the development of their size, number density and volume fraction during aging by applying different analysis techniques in TEM in combination with quantitative microstructural analysis. 3D phase-field simulations of formation and growth of θ´ phase are performed in which the full interfacial, chemical and elastic energy contributions are taken into account. 2D simulations of T_1 phase are also investigated using multi-component diffusion without elasticity. This is a first step toward a complex phase-field study of T_1 phase in the ternary alloy. The comparison between experimental and simulated data shows similar trends. The still unsaturated volume fraction indicates that the precipitates are in the growth stage and that the coarsening/ripening stage has not yet been reached.

Ab-initio study of C and N point defects in the C14-Fe_2Nb phase

A. C. Ladines, R. Drautz, T. Hammerschmidt
Journal of Alloys and Compounds, **693**, 1315-1322 (2017)



Crystal structure of the C14 Laves-phase of Fe_2Nb with Fe atoms in red and Nb atoms in blue. The small spheres indicate possible tetrahedral sites for C and N interstitial atoms.

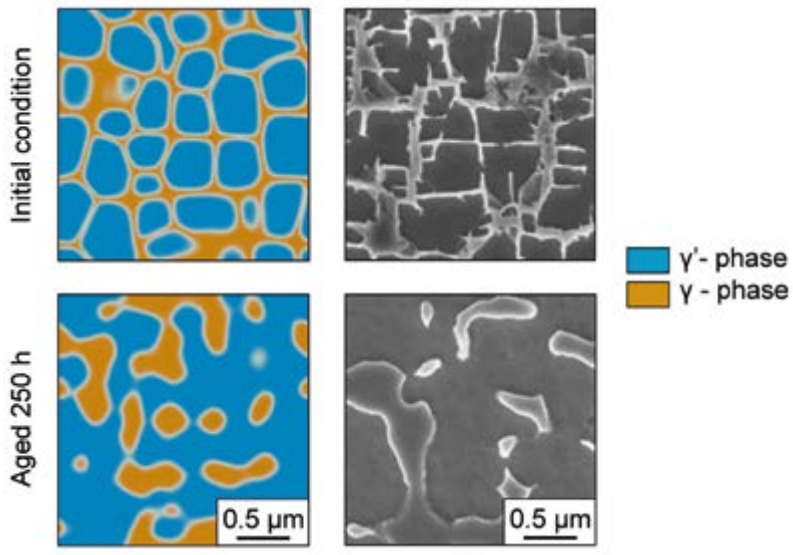
Nb-alloying of steels can lead to the formation of topologically close-packed (TCP) phases, particularly Fe_2Nb Laves and Fe_7Nb_6μ phases. The stability of these TCP phases is strongly affected by the presence of light elements like C and N. We calculate the solution energy of C and N in C14-Fe_2Nb using density functional theory. N shows a strong preference to dissolve in larger interstitial voids while C shows a strong tendency to bind with a neighbouring Nb atom. The computed solution energies suggest N incorporation into Fe_2Nb Laves phases while C is hardly soluble. The N-N interaction in Fe_2Nb is strongly attractive and twice as strong as that of C-C. A comparison to C interstitials in the μ-Fe_7Nb_6 phase shows similar dependence of the solution energy on the atomic environment. In order to aid future work, we additionally provide the coordinates of interstitial sites in all TCP phases (A15, Zr_4Al_3, C14, C15, C36, χ, μ, σ, M, P, δ and R.) in the supplementary material.

Topological phase inversion after long-term thermal exposure of nickel-base superalloys: Experiment and phase-field simulation

J. V. Görler, I. Lopez-Galilea, L. Mujica, O. Shchyglo, W. Theisen, I. Steinbach
Acta Materialia, **124**, 151-158 (2017)

Ni-base superalloys are materials which are designed to resist extreme thermal and mechanical conditions. In this regard, an essential factor is their microstructure consisting of gamma' precipitates embedded in a gamma matrix. The application of superalloys at high temperatures can however induce the topological phase inversion, where the gamma'-phase topologically becomes the matrix phase, resulting in subpar material properties. In this work, the topological inversion is analyzed via experiment and phase-field simulation. The evolution of the microstructure has been quantified in the second generation single crystal Ni-base superalloy ERBO/1, which belongs to the family of CMSX-4, submitted to long-term aging at 1100°C for up to 250 h. Phase-field simulations carried out using a multi phase-field approach deliver insight into the microstructure evolution driven by the loss of coherency of the gamma' precipitates, which is induced by the accumulation of dislocations at the gamma/gamma' interfaces. The obtained simulation results are in good agreement with the experimental results, and indicate that the mechanisms causing the topological inversion are linked to the accommodation of the lattice misfit, which enables coalescence and ripening of gamma' precipitates.

2D cross sections of a 3D simulation as a function of the relative simulation time where gamma'-phase is shown in blue and gamma-phase in orange. SEM In-Lens detector micrographs showing the evolution of the interdentric area after annealing at 1100°C.

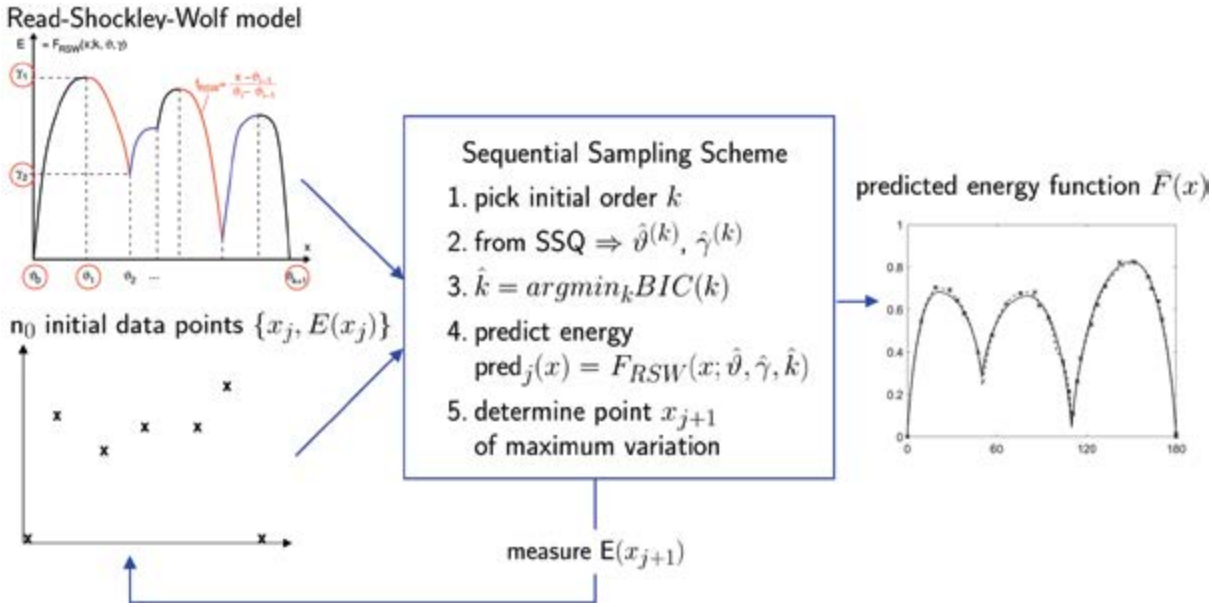


Efficient sampling in materials simulation – Exploring the parameter space of grain boundaries

H. Dette, J. Gösmann, C. Greiff, R. Janisch
Acta Materialia, **125**, 45-155 (2017)

In the framework of materials design there is the demand for extensive databases of specific materials properties. In this work we suggest an improved strategy for creating future databases, especially for extrinsic properties that depend on several material parameters. As an example we choose the energy of grain boundaries as a function of their geometric degrees of freedom. The construction of many existing databases of grain boundary energies in face-centred and body centred cubic metals relied on the a-priori knowledge of the location of important cusps and maxima in the five-dimensional energy landscape, and on an as-densely-as-possible sampling strategy. We introduce two methods to improve the current state of the art. Based on an existing energy model the location and number of the energy minima along which

the hierarchical sampling takes place is predicted from existing data points without any a-priori knowledge, using a predictor function. Furthermore we show that in many cases it is more efficient to use a sequential sampling in a "design of experiment" scheme, rather than sampling all observations homogeneously in one batch. This sequential design exhibits a smaller error than the simultaneous one, and thus can provide the same accuracy with fewer data points. The new strategy should be particularly beneficial in the exploration of grain boundary energies in new alloys and/or non-cubic structures.



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3D discrete dislocation dynamics study of creep behavior in Ni-base single crystal superalloys by a combined dislocation climb and vacancy diffusion model

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

Journal of the Mechanics and Physics of Solids, **102**, 209-223 (2017)

A three-dimensional (3D) discrete dislocation dynamics (DDD) creep model is developed to investigate creep behavior under uniaxial tensile stress along the crystallographic [001] direction in Ni-base single crystal superalloys, which takes explicitly account of dislocation glide, climb and vacancy diffusion, but neglects phase transformation like rafting of γ-precipitates. The vacancy diffusion model takes internal stresses by dislocations and mismatch strains into account and it is coupled to the dislocation dynamics model in a numerically efficient way. This model is helpful for understanding the fundamental creep mechanisms in superalloys and clarifying the effects of dislocation glide and climb on creep deformation. In cases where the precipitate cutting rarely occurs, e.g. due to the high anti-phase boundary energy and the lack of superdislocations, the dislocation glide in the γ-matrix and the dislocation climb along the γ/γ′ interface dominate plastic deformation. The simulation results show that a high temperature or a high stress both promote dislocation motion and multiplication, so as to cause a large creep strain. Dislocation climb

accelerated by high temperature only produces a small plastic strain, but relaxes the hardening caused by the filling γchannels and lets dislocations further glide and multiply. The strongest variation of vacancy concentration occurs in the horizontal channels, where more mixed dislocations exit and tend to climb. The increasing internal stresses due to the increasing dislocation density are easily overcome by dislocations under a high external stress that leads to a long-term dislocation glide accompanied by multiplication.

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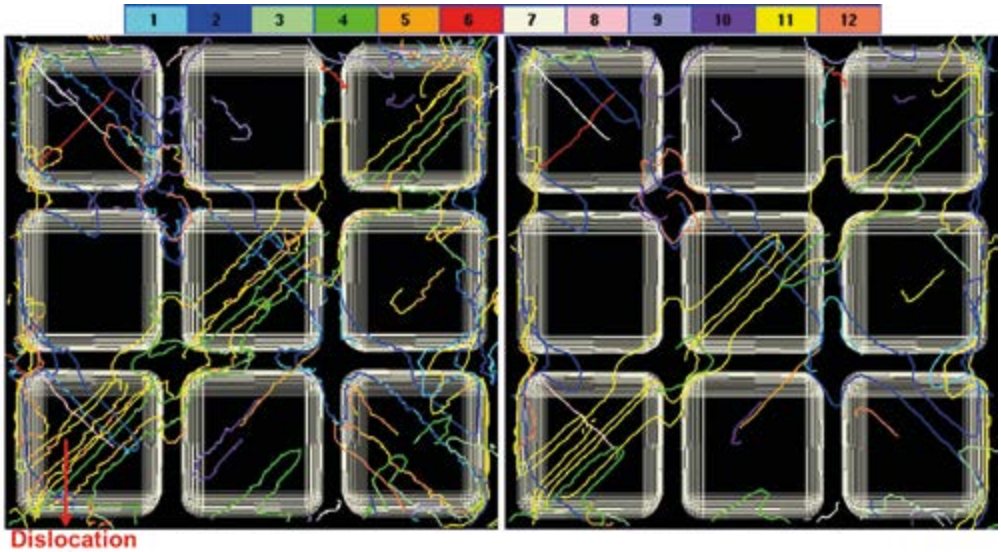
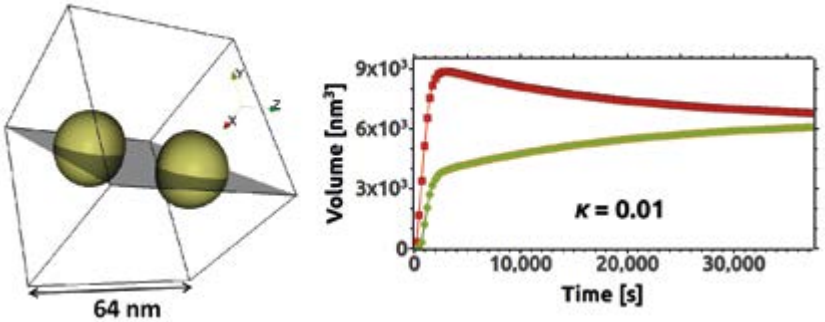


Inverse ripening and rearrangement of precipitates under chemomechanical coupling

R. Darvishi Kamachali, C. Schwarze

Computational Materials Science, **130**, 292-296 (2017)



In the presence of chemomechanical coupling effect, inverse ripening occurs in which the smaller precipitate grows at the expense of the larger one. The size evolution and configuration of two evolving precipitates are shown in the figure. The precipitates have different initial size.

A coupling between diffusional and mechanical relaxation raised from composition-dependent elastic constants, and its effects on the evolution of precipitates with finite misfit strain are investigated. Inverse ripening has been observed where smaller precipitate grows at the expense of a larger one. This occurs due to fluxes generated under elastically-strained solute gradients around precipitates that scales with $(R/r)^6$ where R and r are the precipitate radius and the radial coordinate, respectively. Both isotropic and anisotropic dependency of elastic constants on the composition were considered. The latter leads to the emergence of new patterns of elastic anisotropy and rearrangement of precipitates in the matrix.

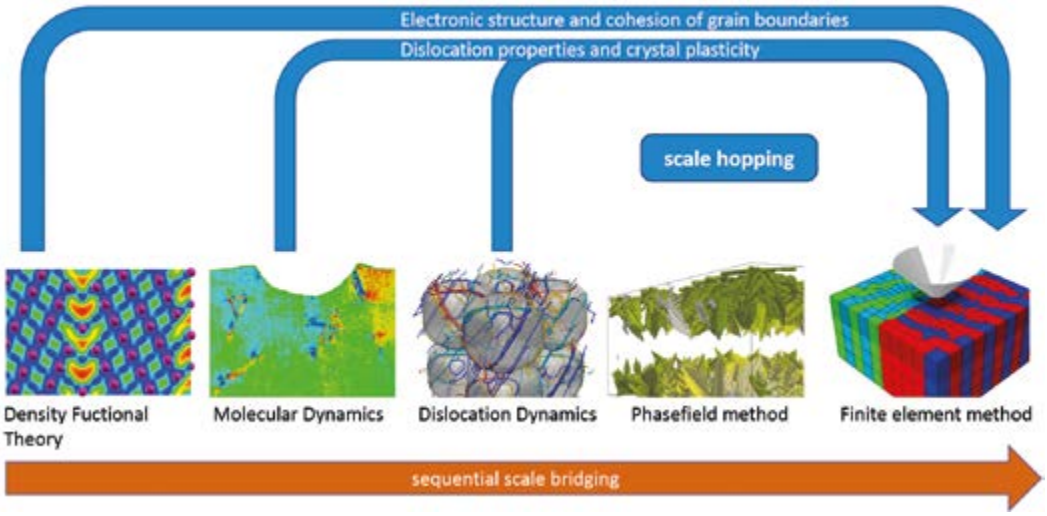
Vom Atom zum Bauteil und zurück

A. Hartmaier

Physik in unserer Zeit, **48**, 90-197 (2017)

The American "Materials Genome Initiative" has the goal of describing materials across different length and time scales. European research also wants to successfully link physical ab initio models for the atomic scale with meso- and macroscopic models of materials in order to design materials in a targeted manner. This is a challenge because of limited computer performance.

Die amerikanische "Materials Genome Initiative" hat zum Ziel, Werkstoffe skalenüberbrückend zu beschreiben. Auch die europäische Forschung will physikalische Ab-inito-Modelle für die atomare Skala erfolgreich mit meso- und makroskopischen Modellen der Material- und Werkstoffwissenschaften verknüpfen, um Werkstoffe gezielt designen zu können. Das ist allein schon wegen der beschränkten Computerleistung eine Herausforderung.

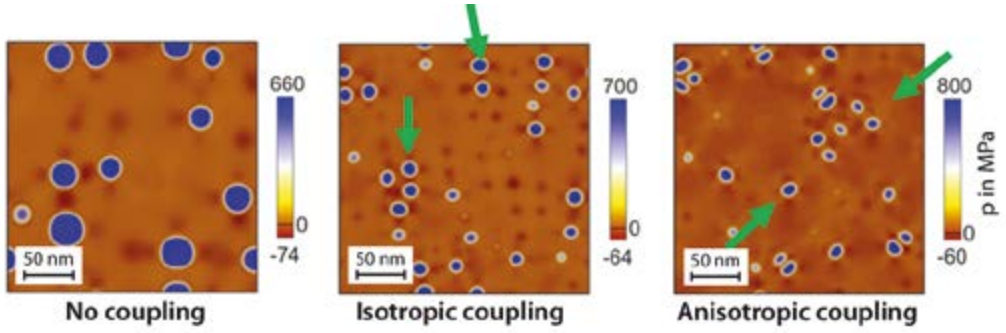


Phase-field study of ripening and rearrangement of precipitates under chemomechanical coupling

C. Schwarze, A. Gupta, T. Hickel, R. Darvishi Kamachali
Physical Review B, **95**, 174101 (2017)

We investigate the evolution of large number of δ′coherent precipitates from a supersaturated Al-8 at.% Li alloy using large-scale phase-field simulations. A chemomechanical cross-coupling between mechanical relaxation and diffusion is taken into account by considering the dependence of elastic constants of the matrix phase onto the local concentration of solute atoms. The elastic constants as a function of solute concentration have been obtained using density functional theory calculations. As a result of the coupling, inverse ripening has been observed where the smaller precipitates grow at the expense of the larger ones. This is due to size-dependent concentration gradients existing around the precipitates. At the same time, precipitates rearrange themselves as a consequence of minimization of the total elastic energy of the system. It is found that the anisotropy of the chemomechanical coupling leads to the formation of new patterns of elasticity in the matrix thereby resulting in new alignments of the precipitates.

The bilateral chemomechanical coupling results is stabilization of precipitates and emergence of new patterns of elasticity in the system. In the Figure 2D cross-sections of 3D phase-field simulations are shown. Different coupling values lead to different alignment of precipitates (green arrows).



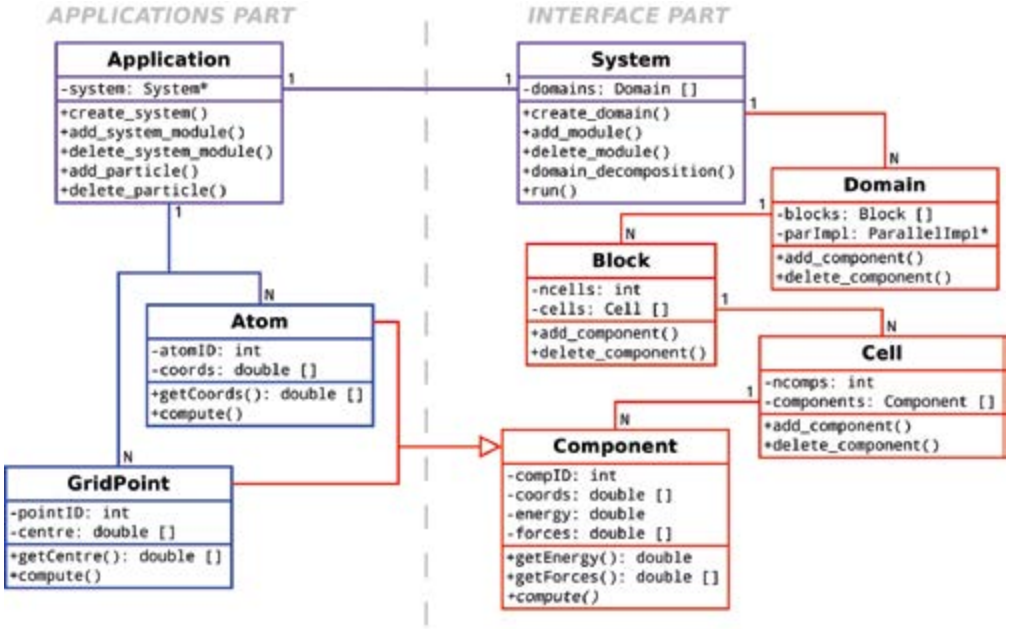
Towards a flexible cell-based framework for parallel scale-bridging simulations in materials science: A first case study

C. Teijeiro Barjas, H. Ganesan, R. Halver, W. Homberg, G. Sutmann
Proceedings of the 5th International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering, Hungary, Paper 24 (2017)

The use of different simulation methods in materials science is necessary to provide accurate and efficient solutions for each specific time and length scale: e.g., an accurate description of atom properties requires a high amount of information, but the analysis of microstructures takes higher level descriptions of compounds. Nevertheless, the implementation of scale-bridging techniques requires specific modelling efforts in order to transfer information between different approaches, as well as suitable computational tools that facilitate the connection between simulations. In this aspect, the present work describes the first steps in the development of a parallel cell-based framework for the optimised execution of a wide variety of simulations. The proposed framework acts as a skeleton that defines parallel simulations by using the concepts of domains, cells and components as its central constructs, and also incorporating further functionalities in a modular way (e.g. load balancing algorithms). The correct management of the framework has been tested with a first

example, which consist in the coupling of molecular dynamics with Monte Carlo to show the segregation of carbon (C) in a defect bcc iron (Fe) structure. The existing code is connected to the framework to obtain a parallel execution with domain decomposition and load balancing. The test results give a good perspective of the current potential of the simulation framework, and also help to guide the future developments and improvements.

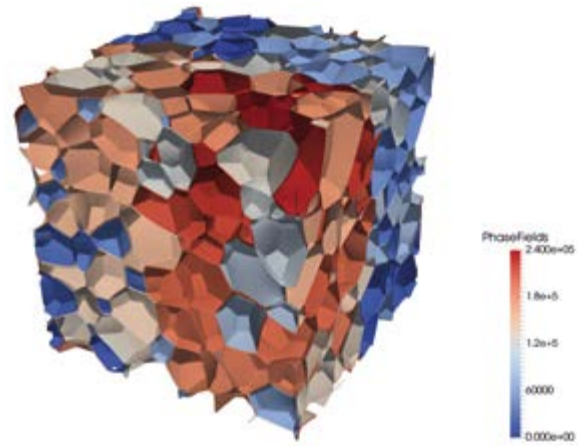
Connection between an application and the simulation framework.



Parallel multiphase field simulations with OpenPhase

M. Tegeler, O. Shchyglo, R. Darvishi Kamachali, A. Monas, I. Steinbach, G. Sutmann

Computer Physics Communications, **215**, 173-187 (2017)



Simulation of normal grain growth with 240000 initial grains.

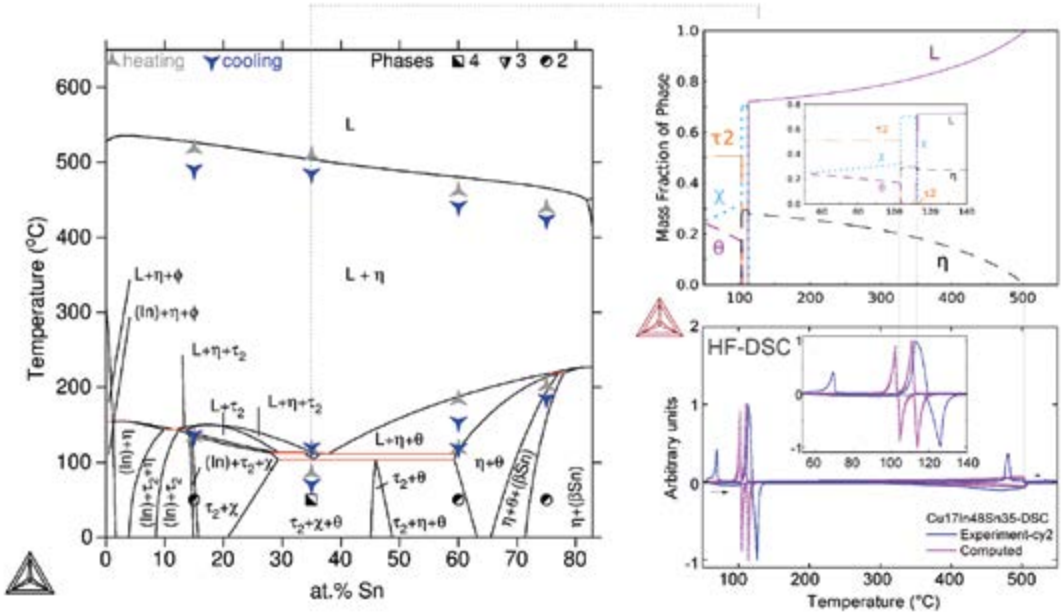
The open-source software project OpenPhase allows the three-dimensional simulation of microstructural evolution using the multiphase field method. The core modules of OpenPhase and their implementation as well as their parallelization for a distributed-memory setting are presented. Especially communication and load-balancing strategies are discussed. Synchronization points are avoided by an increased halo-size, i.e. additional layers of ghost cells, which allow multiple stencil operations without data exchange. Load-balancing is considered via graph-partitioning and sub-domain decomposition. Results are presented for performance benchmarks as well as for a variety of applications, e.g. grain growth in polycrystalline materials, including a large number of phase fields as well as Mg-Al alloy solidification.

Multiphase characterization of Cu-In-Sn alloys with 17 at.% Cu and comparison with calculated phase equilibria

S. Tumminello, N. Del Negro, C. Carrascal, S. G. Fries, P. R. Alonso, S. Sommadossi
Journal of Phase Equilibria and Diffusion, **38**, 276-287 (2017)

Cu-In-Sn alloys are among the suggested materials to replace Pb-Sn alloys traditionally used in joining processes by the electronic industry. Thorough thermodynamic understanding is required for the selection/design of adequate and efficient alloys for specific applications. Understanding the effects that high cost elements such as In have on microstructure and phase stability is imperative for industrial use. In this work ternary alloys were prepared by melting high purity elements (5N) for selected compositions of the 17 at.% Cu isopleth, and cooling down to reproduce process conditions. Chemical composition was determined using scanning electron microscopy equipped with electron probe microanalysis. Measurements of transition temperatures were done by heat-flux differential scanning calorimetry. We present a comprehensive comparison between our experimental results and phase diagram calculations using Liu et al. (J. Electron Mater 30:1093, 2001) thermodynamic description based in the CALPHAD method, available in the literature.

Results for CALPHAD simulations and HF-DSC simulations and experimental measurements for Cu-In-Sn alloys.



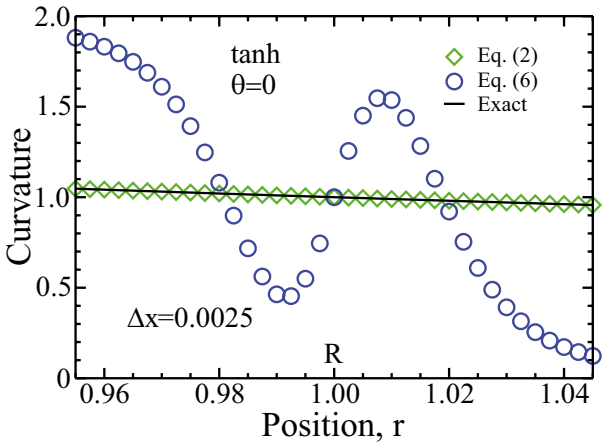
CALPHAD ⟶ DF- DSC simulation ⟷ HF - DSC measurements

On the numerical evaluation of local curvature for diffuse interface models of microstructure evolution

S. Vakili, I. Steinbach, F. Varnik

Procedia Computer Science, **108**, 1852-1862 (2017)

Within diffuse interface models for multiphase problems, the curvature of the phase boundary can be expressed as the difference of two terms, a Laplacian and a second, gradient, term of the diffuse interface variable, ø. In phase field simulations of microstructure evolution, the second term is often replaced by f′(ø) = df/dø, where f(ø) is the potential function in the free energy functional of the underlying physical model. We show here that this replacement systematically deteriorates the accuracy in local curvature evaluation as compared to a discretized evaluation of the second term. Analytic estimates reveal that the discretization errors in the Laplacian and in the second term have roughly the same spatial dependence across the interface, thus leading to a cancellation of errors in k. This is confirmed in a test case, where the discretization error can be determined via comparison to the exact solution. If, however, the second term is replaced by a quasi exact expression, the error in Δø enters k without being compensated and can obscure the behavior of the local curvature. Due to the antisymmetric variations of this error term, approaches using the average curvature, as obtained from an integral along the interface normal, are immune to this problem.

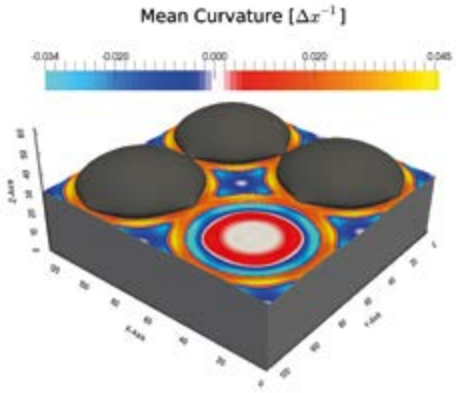


Curvature evaluated using the proposed error cancellation scheme (red diamonds) and the standard approach (blue circles) for the case of a double well potential. The solid line shows the exact result for a radial phase field, reprenting a two dimensional disc of radius R=1.

Multi-phase-field model for surface/phase-boundary diffusion

R. Schiedung, R. Darvishi Kamachali, I. Steinbach, F. Varnik
Physical Review E, **96**, 12801 (2017)

The multi-phase-field approach is generalized to treat capillarity-driven diffusion parallel to the surfaces and phase boundaries, i.e., the boundaries between a condensed phase and its vapor and the boundaries between two or multiple condensed phases. The effect of capillarity is modeled via curvature dependence of the chemical potential whose gradient gives rise to diffusion. The model is used to study thermal grooving on the surface of a polycrystalline body. Decaying oscillations of the surface profile during thermal grooving, postulated by Hillert long ago but reported only in few studies so far, are observed and discussed. Furthermore, annealing of multi-nanoclusters on a deformable free surface is investigated using the proposed model. Results of these simulations suggest that the characteristic craterlike structure with an elevated perimeter, observed in recent experiments, is a transient nonequilibrium state during the annealing process.

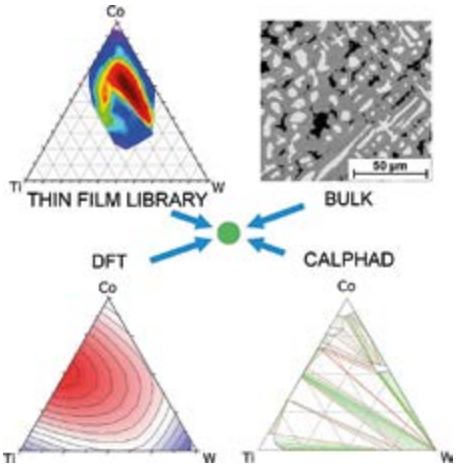


The entrenching of multiple nanoclusters α into a deformable surface β by surface and phase-boundary diffusion.

Identification of a ternary μ-phase in the Co-Ti-W system – An advanced correlative thin-film and bulk combinatorial materials investigation

D. Naujoks, Y. M. Eggeler, P. Hallensleben, J. Frenzel, S. G. Fries, M. Palumbo, J. Koßmann, T. Hammerschmidt, J. Pfetzing-Micklich, G. Eggeler, E. Spiecker, R. Drautz, A. Ludwig
Acta Materialia, **138**, 100-110 (2017)

The formation of a ternary μ-phase is documented for the system Co-Ti-W. The relevant compositional stability range is iden tified by high-throughput energy dispersive x-ray spectroscopy, electrical resistance and x-ray diffraction maps from a thin-film materials library (1 μm thickness). Bulk samples of the identified compositions were fabricated to allow for correlative film and bulk studies. Using analytical scanning and transmission electron microscopy, we demonstrate that in both, thin film and bulk samples, the D85 phase (μ-phase) coexists with the C36-phase and the A2-phase at comparable average chemical compositions. Young's moduli and hardness values of the μ-phase and the C36-phase were determined by nanoindentation. The trends of experimentally obtained elastic moduli are consistent with density functional theory (DFT) calculations. DFT analysis also supports the experimental findings, that the μ-phase can solve up to 18 at.% Ti. Based on the experimental and DFT results it is shown that CALPHAD modeling can be modified to account for the new findings.



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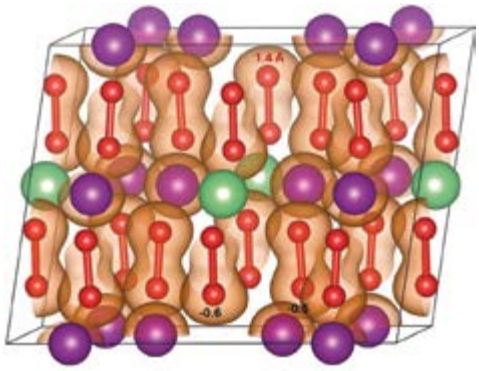
Oxygen activity and peroxide formation as charge compensation mechanisms in L_2MnO_3

A. Marusczyk, J. Albina, T. Hammerschmidt, R. Drautz, T. Eckl, G. Henkelman
Journal of Materials Chemistry A, **5**, 15183-15190 (2017)

In the search for high energy density battery materials, over-lithiated transition metal oxides have attracted the attention of many researchers worldwide. There is, however, no consensus regarding the underlying mechanisms that give rise to the large capacities and also cause the electrochemical degradation upon cycling. As a key component and prototype phase, Li_2MnO_3 is investigated using density functional theory. Our calculations show that hole doping into the oxygen bands is the primary charge compensation mechanism in the first stage of delithiation. Upon further delithiation, there is an energetic driving force for peroxide formation with an optimal number of peroxide dimers that is predicted as a function of lithium concentration. Unlike the defect-free phases, the peroxide structures are highly stable, which leads to two competing mechanisms for charge compensation: (i) oxygen loss and densification at the surface and (ii) peroxide formation in the bulk. Our results show that both have a detrimental effect on the electrochemical performance and therefore the stabilization of oxygen in the crystal lattice is vital for the development of high energy cathode materials. The insights into the origin and implications of peroxide formation open the door for a more profound understanding of the degradation mechanism and how to counteract it.

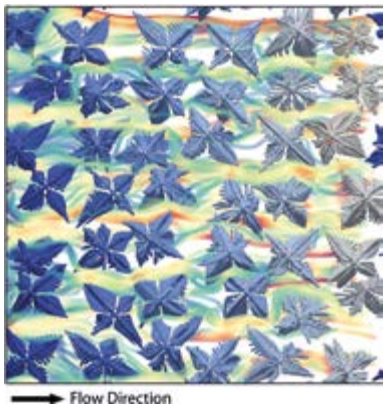


Formation of peroxides in partially delithiated Li_2MnO_3 as obtained from DFT calculations.

Effect of microstructure during dendritic solidification on melt flow: A phase-field lattice-Boltzmann study

M. Tegeler, A. Monas, O. Shchyglo, I. Steinbach, F. Varnik
Proceedings of the 6th Decennial International Conference on Solidification Processing, 280-283 (2017)

In this work, we present a combined phase-field lattice-Boltzmann study of the time evolution of permeability in a Mg-5%Al-cast alloy during its solidification. The phase-field method (PF) is used to determine dendritic microstructures close to the columnar to equiaxed transition under purely diffusive conditions. The fluid flow through the thus obtained microstructures is investigated using the lattice-Boltzmann method (LBM). First, the applicability of the Darcy law is demonstrated by showing that the effective volumetric flow rate across the microstructure is linearly proportional to the applied driving force. This allows us to introduce the concept of permeability in the context of microstructure evolution. In a second step, permeability is determined at different stages of solidification. Our results quantify the decrease of permeability during solidification. These studies underline the maturity of the hybrid PF-LBM approach in dealing with complex phenomena.



View from the top of the simulation domain depicting stream lines of a flow through a channel along dendrites.

On the evolution of cast microstructures during processing of single crystal Ni-base superalloys using a Bridgman seed technique

P. Hallensleben, H. J. Schaar, P. Thome, N. Jöns, A. Jafarizadeh, I. Steinbach, G. Eggeler, J. Frenzel
Materials & Design, **128**, 98-111 (2017)

The present work takes a new look at a modified Bridgman process (Bridgman seed technique, BST) for the production of laboratory Ni-base single crystal (SX) superalloy cylinders of 12/120 mm diameter/length. This type of specimen is needed to perform inexpensive parametric studies for the development of new SX and for understanding the evolution of microstructures during SX casting. During melting, the seed partially melts back. The elementary segregation processes cause a so far unknown type of constitutional heating/cooling. Competitive growth eventually establishes a constant average dendrite spacing. In the present work it is documented how this dendrite spacing varies in one cylindrical ingot, and how it scatters when a series of SX ingots is produced. This type of information is scarce. The calculated temperature gradient across the solid/liquid interface (calculated by FEM) is in excellent agreement with predictions from the Kurz-Fisher equation which yields a dendrite spacing based on the experimental withdrawal rate and the microstructurally determined average dendrite spacing. The presence of small angle grain boundaries on cross sections which were taken perpendicular to the solidification direction can be rationalized on the basis of small deviations from the ideal growth directions of individual primary dendrites.

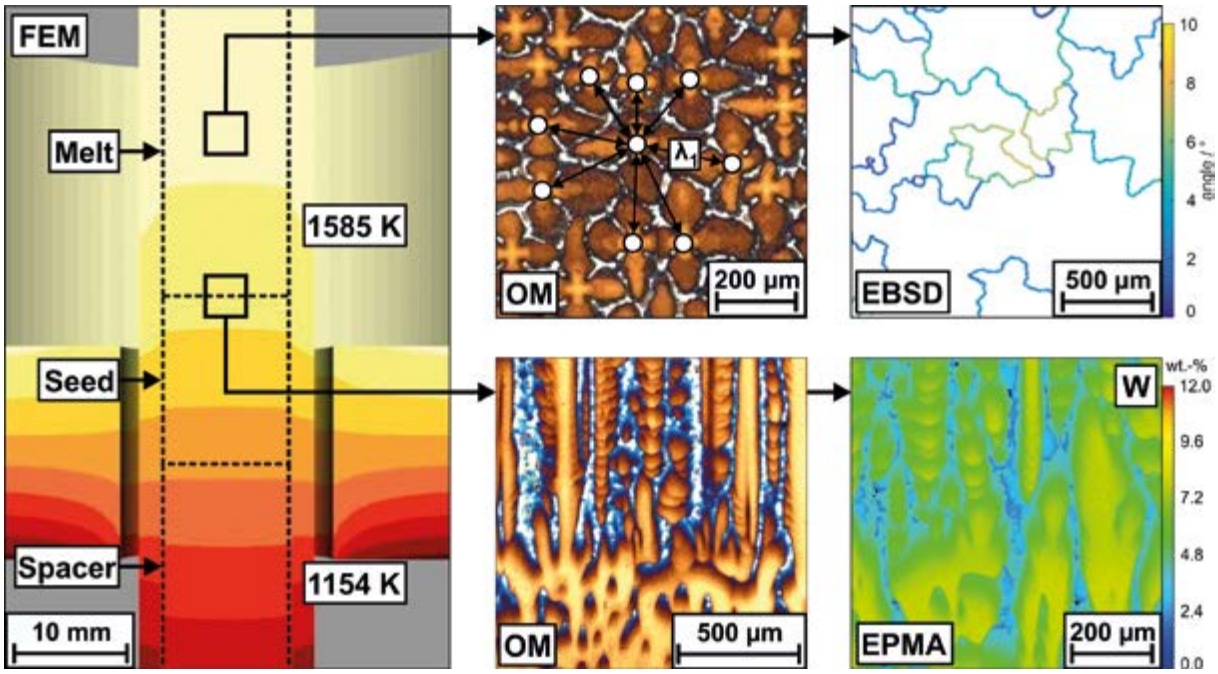


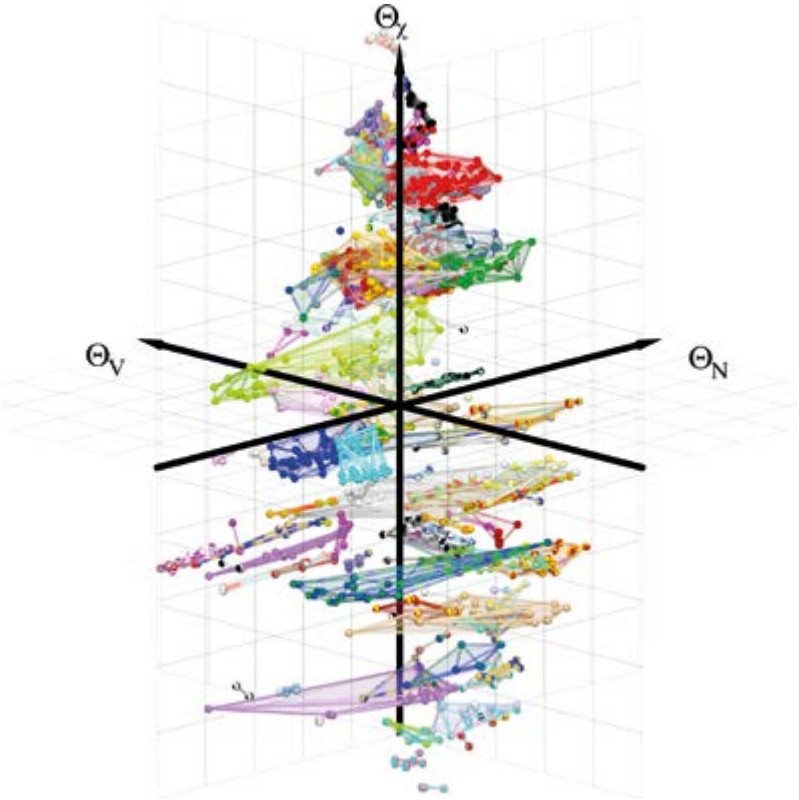
Illustration of the calculated temperature fields in the melt feedstock with the corresponding experimentally observed dendritic microstructures (OM = Optical Microscope).

Structure map including off-stoichiometric and ternary sp-d-valent compounds

T. Hammerschmidt, A. Bialon, R. Drautz

Modelling and Simulation in Materials Science and Engineering, **25**, 74002 (2017)

Structure maps predict the crystal structure of a compound from the knowledge of constituent elements and chemical composition. We recently developed a highly predictive, three-dimensional structure map for stoichiometric binary sp-d-valent compounds. Here we show that the descriptors of this structure map are transferable to off-stoichiometric compounds with similarpredictive power. We furthermore demonstrate that the descriptors are suitable for ternary prototypes. In particular, we construct a three-dimensional structure map for 129 prototypical crystal structures for ternary compounds. The crystal structure is predicted correctly with a probability of 78%. With a confidence of 95% the correct crystal structure is among the three most likely crystal structures predicted by the structure map.

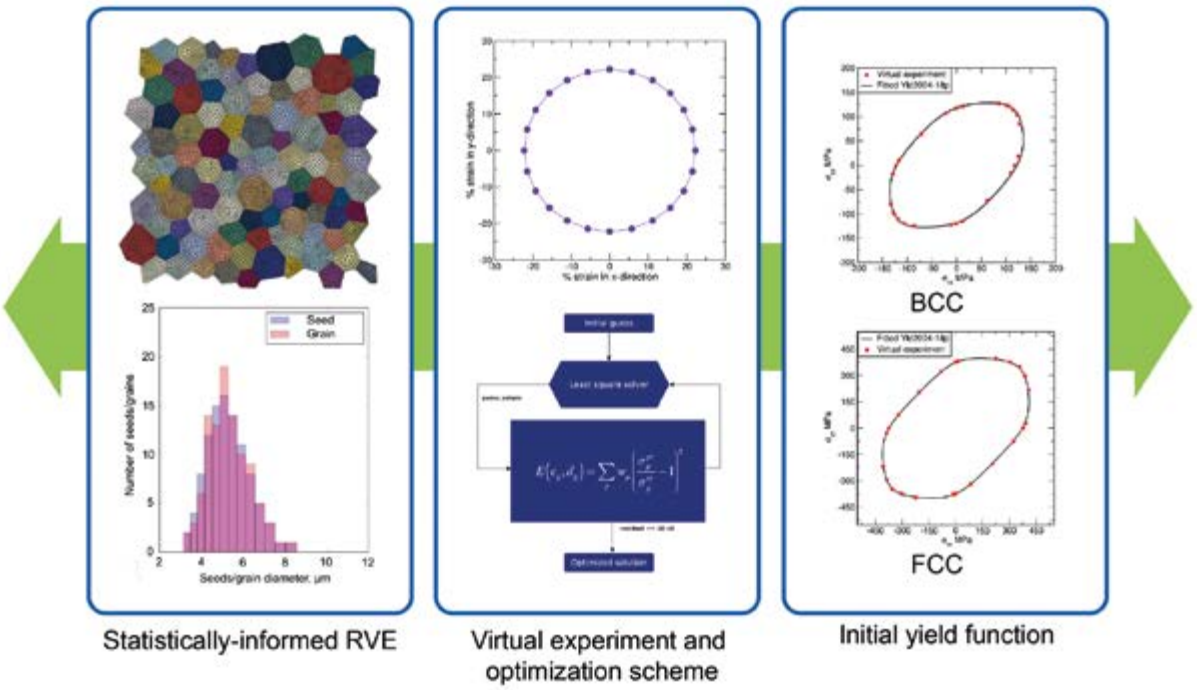


Three-dimensional structure map for the prediction of the crystal structure of ternary compounds. The descriptors are based on the number of valence electrons N, the atomic volume V and the electro-negativity X of the constituent elements. The coloured polyhedrons correspond to different crystal structures.

Micromechanical modeling approach to derive the yield surface for BCC and FCC steels using statistically informed microstructure models and nonlocal crystal plasticity

N. Vajragupta, S. Ahmed, M. Boeff, A. Ma, A. Hartmaier
Physical Mesomechanics, **20**, 100-108 (2017)

In order to describe irreversible deformation during metal forming processes, the yield surface is one of the most important criteria. Because of their simplicity and efficiency, analytical yield functions along with experimental guidelines for parameterization become increasingly important for engineering applications. However, the relationship between most of these models and microstructural features are still limited. Hence, we propose to use micromechanical modeling, which considers important microstructural features, as a part of the solution to this missing link. This study aims at the development of a micromechanical modeling strategy to calibrate material parameters for the advanced analytical initial yield function Barlat YLD 2004-18p. To accomplish this, the representative volume element is firstly created based on a method making use of the statistical description of microstructure morphology as input parameter. Such method couples particle simulations to radical Voronoi tessellations to generate realistic virtual microstructures as representative volume elements. Afterwards, a nonlocal crystal plasticity model is applied to describe the plastic deformation of the representative volume element by crystal plasticity finite element simulation. Subsequently, an algorithm to construct the yield surface based on the crystal plasticity finite element simulation is developed. The primary objectives of this proposed algorithm are to automatically capture and extract the yield loci under various loading conditions. Finally, a nonlinear least square optimization is applied to determine the material parameters of Barlat YLD2004-18p initial yield function of representative volume element, mimicking generic properties of bcc and fcc steels from the numerical simulations.

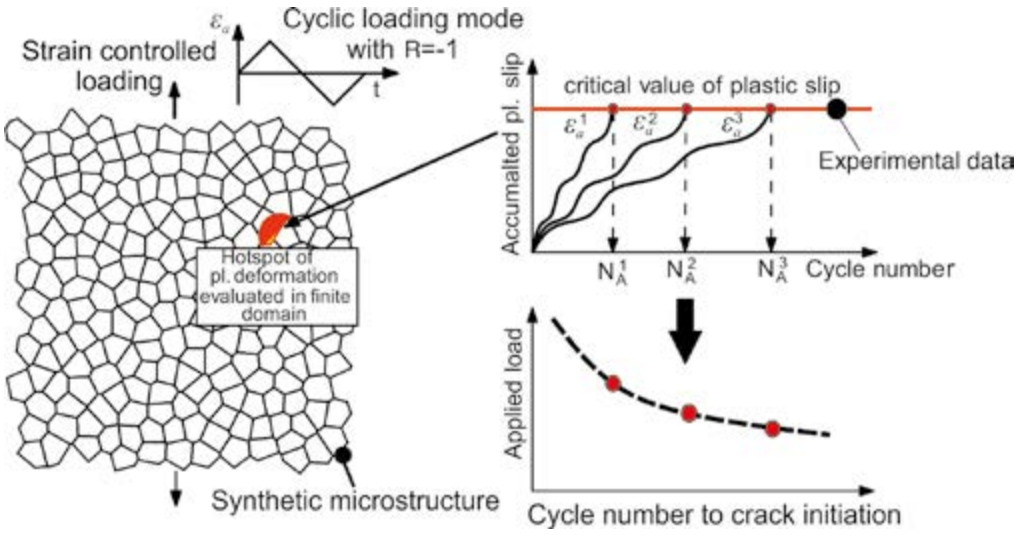


Schematic diagram for the micromechanical modeling approach to derive an advanced initial yield surface.

Micromechanical modeling of fatigue crack initiation in polycrystals

M. Boeff, H. u. Hassan, A. Hartmaier
Journal of Materials Research, **32**, 4375-4386, (2017)

Fatigue is an important mechanism for the failure of components in many engineering applications and a significant proportion of the fatigue life is spent in the crack initiation phase. Although a large number of research work addresses fatigue life and fatigue crack growth, the problem of modeling crack initiation remains a major challenge in the scientific and engineering community. In the present work, a micromechanical model is developed and applied to study fatigue crack initiation. In particular, the effect of different hardening mechanisms on fatigue crack initiation is investigated. To accomplish this, a model describing the evolution of the particular dislocation structures observed under cyclic plastic deformation is implemented and applied on randomly generated representative microstructures to investigate fatigue crack initiation. Finally, a method is presented to calculate the S–N curve for the polycrystalline materials. With this work, it is demonstrated how the micromechanical modeling can support the understanding of damage and failure mechanisms occurring during fatigue.



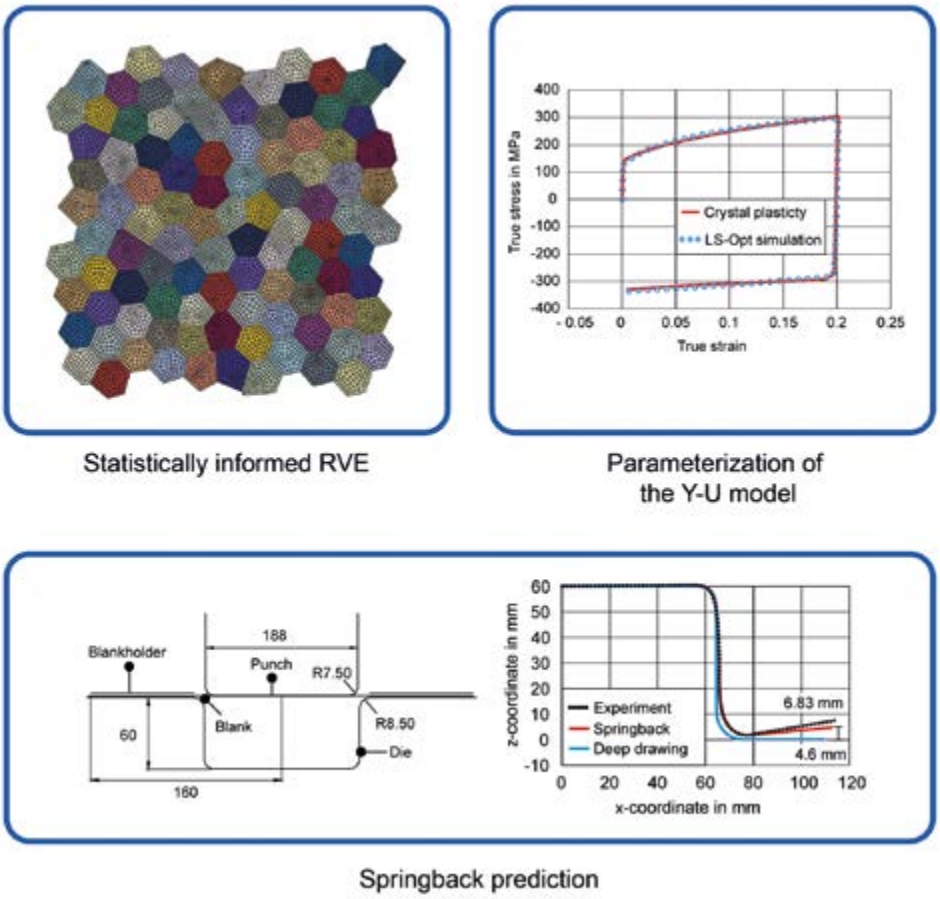
Schematic diagram of the algorithm for the estimation of the lifetime for fatigue crack initiation.

Towards prediction of springback in deep drawing using a micromechanical modeling scheme

N. Vajragupta, H. u. Hassan, A. Hartmaier
Procedia Engineering, **207**, 60-65 (2017)

Deep drawing is one of the most commonly used sheet metal forming processes, which can produce metal parts at a high rate. One of the major problems in deep drawing is springback, which is mainly elastic deformation occurring when the tool is removed. The focus of this work is the prediction of springback in deep drawing for DC04 steel using a micromechanical modeling scheme. A novel method is used for the characterization of material that leads to cyclic stress-strain curve. Simulations are performed with the Yoshida Uemori (YU) model for the prediction of springback for a U draw-bend geometry. The maximum deviation between the geometries of experiment and the springback simulation for hat geometry is 2.2 mm. It is shown that this micromechanical modeling scheme allows us to relate the influence of the microstructure to the springback prediction.

Micromechanical scheme to predict springback in deep drawing.

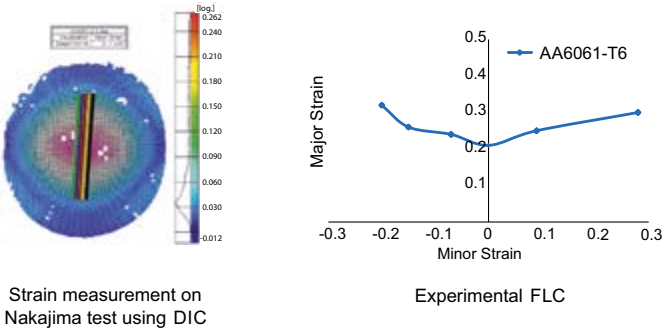


Comparison of deep drawability of AA5754-H22 and AA6061-T6 aluminum alloys for automotive applications

M. Ipekoglu, O. Erbas, H. u. Hassan

Materials Testing, Materialprüfung, **59**, 1003-1008 (2017)

Being one of the most commonly applied sheet metal forming processes in automotive industry, deep drawing technologies are challenged by the concerns of global warming for higher fuel economy requirements in the recent years. To reduce the weight of the vehicles in order to obtain fuel economy, lighter and safer materials are used in automotive industry. Aluminum alloys, due to their low density compared to steels, are an important group of materials, in particular for lightweight construction of vehicles. In this study, two different aluminum alloys, namely AA5754-H22 and AA6061-T6, are evaluated for their potential use in nonload bearing applications in commercial vehicles by comparing their deep drawability characteristics. For this purpose, they are characterized by uniaxial tensile and Nakajima tests. In the next step, the deep drawing experiments are performed under different levels of blankholder force. The distance of the cup center to the edge of the die is also evaluated to investigate the formability of the designed cup for commercial use and to obtain the required product quality.



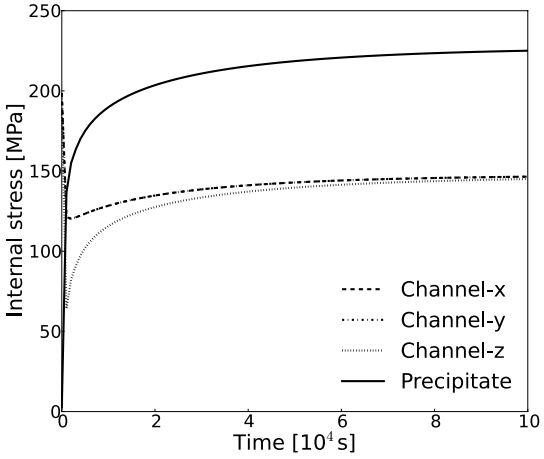
Strain measurement on Nakajima test using digital image correlation and the determination of forming limit curve (FLC).

Numerically efficient microstructure-based calculation of internal stresses in superalloys

S. Gao, U. Gogilan, A. Ma, A. Hartmaier

Modelling and Simulation in Materials Science and Engineering, **26**, 25001 (2017)

According to the classical Eshelby inclusion problem, we introduce a new linear relation to calculate internal stresses in γ/γ′ microstructures of superalloys via an effective stiffness method. To accomplish this, we identify regions with almost uniform deformation behavior within the microstructure. Assigning different eigenstrains to these regions results in a characteristic internal stress state. The linear relation between eigenstrains and internal stresses, as proposed by Eshelby for simpler geometries, is shown to be a valid approximation to the solution for complex microstructures. The fast Fourier transformation method is chosen as a very efficient numerical solver to determine the effective stiffness matrix. Numerical validation shows that this generalized method with the effective stiffness matrix is efficient to obtain appropriate internal stresses and that it can be used to consider the influence of internal stresses on plasticity and creep kinetics in superalloys.



The von Mises internal stresses in one element for the cubic γ′ precipitate as a function of time under uniaxial tensile load of 300 MPa in z-direction. (c) IOP Publishing. Reproduced with permission. All rights reserved.

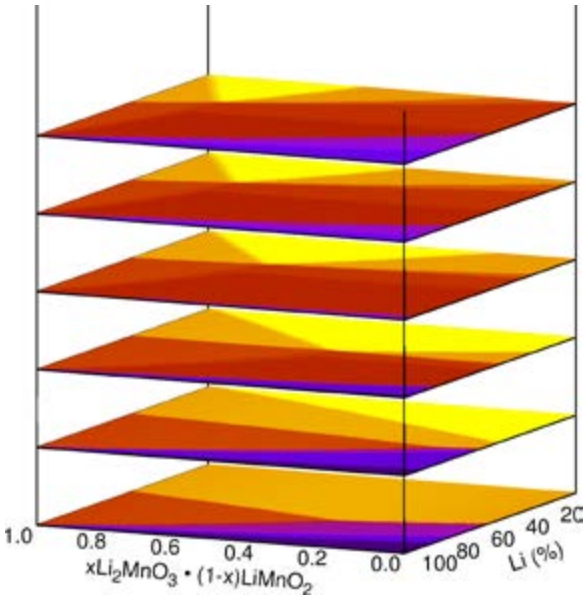
12. Research Highlights

2018

Finite-temperature property-maps of Li-Mn-Ni-O cathode materials from ab initio calculations

J. Albina, A. Marusczyk, T. Hammerschmidt, T. Eckl, R. Drautz
Journal of Materials Chemistry A, **6**, 5687-5694 (2018)

We report first-principles calculations for determining the phase relationships in multi-component cathode materials. We investigate the effect of delithiation on the phase stability, chemical potential, and open circuit voltage for a selection of cathode materials based on Li-Mn-Ni oxides at various temperatures. Entropic contributions are included by calculating the phonon frequencies in the harmonic approximation. The open circuit voltage in multi-component systems is estimated by a convex hull approach. We confirm that spinel-like phases are predominant during the charging process of layered Li-Mn-O cathode materials and that the addition of Ni reduces the spinel content. The analysis of phase stability upon delithiation suggests that the Li_2MnO_3 component in the Li_2MnO_3·$Li(Mn,Ni)O_2$ electrode material should not exceed 60% and that the amount of Ni in the $LiMnO_2$ component should be above 40 at% for minimizing spinel-type phase formation and minimizing oxygen formation. Using the computed structural stability at room temperature, we derive property maps for the design of Li-Mn-Ni-O cathode materials.

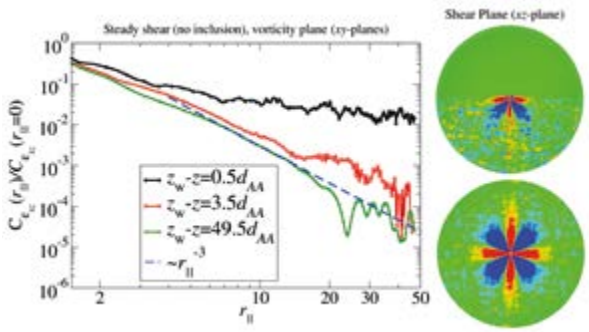


Finite-temperature property map of electrochemical properties for the design of Li-Mn-Ni-O cathode materials.

Wall effects on spatial correlations of non-affine strain in a 3D model glass

M. R. Hassani, P. S. Engels, F. Varnik
EPL Journal, **121**, 18005 (2018)

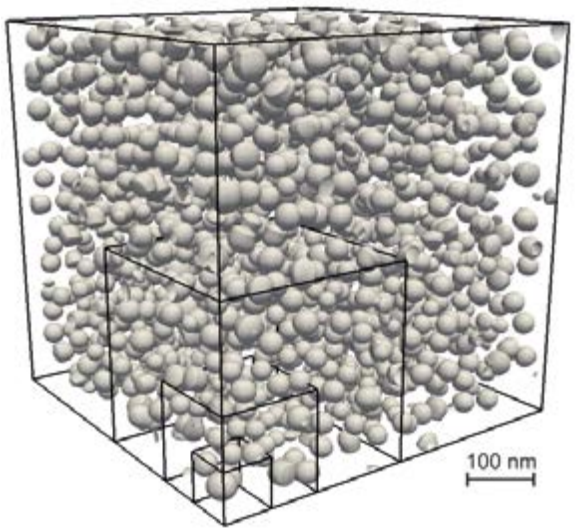
Effects of hard planar walls with a particle scale roughness on the spatial correlations of non-affine strain in amorphous solids are investigated via molecular dynamics simulations. When determined within layers parallel to the wall plane, normalized non-affine strain correlations are enhanced within layers closer to the wall. The amplitude of these correlations, on the other hand, is found to be suppressed by the wall. While the former is connected to the effects of a hard boundary on the continuum mechanics scale, the latter is attributed to molecular scale wall effects on the size of the region (nearest-neighbor cage), explored by particles on intermediate times scales.



Normalized correlations of non-affine shear strain versus distance between two rearrangement events. The color maps on the right show correlations within the xz-plane close to the wall (upper image) and far away from it (lower image).

Computationally efficient phase-field simulation studies using RVE sampling and statistical analysis

C. Schwarze, R. Darvishi Kamachali, C. Mießen, M. Tegeler, L. Barrales-Mora, I. Steinbach, G. Gottstein, M. Kühbach
Computational Materials Science, **147**, 204-216 (2018)



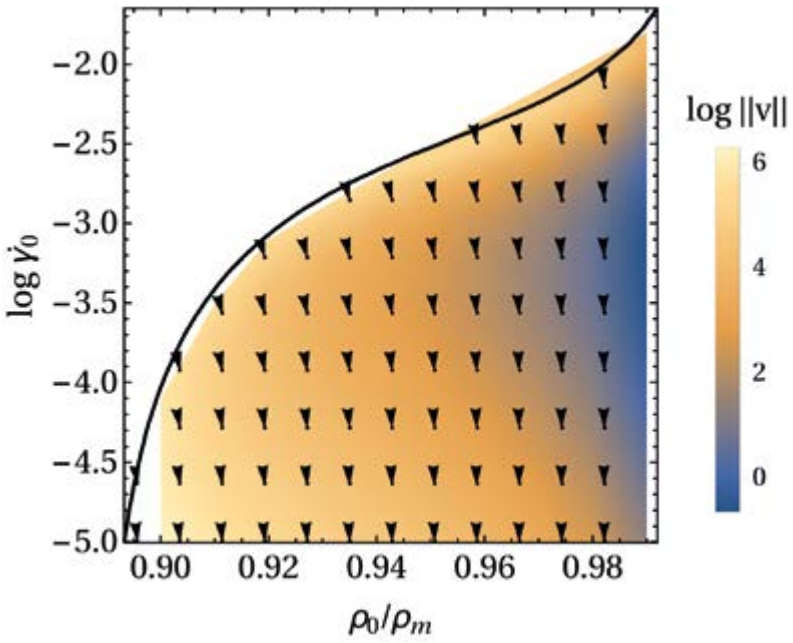
Snapshot of the particle distribution in the reference RVE (5123 nm³). The simulation box contains subdivisions of 2563 nm³, 1283 nm³, and 643 nm³.

For large-scale phase-field simulations, the trade-off between accuracy and computational cost as a function of the size and number of simulations was studied. For this purpose, a large reference representative volume element (RVE) was incrementally subdivided into smaller solitary samples. We have considered diffusion-controlled growth and early ripening of δ'(Al_3Li)) precipitate in a model Al-Li system. The results of the simulations show that decomposition of reference RVE can be a valuable computational technique to accelerate simulations without a substantial loss of accuracy. In the current case study, the precipitate number density was found to be the key controlling parameter. For a pre-set accuracy, it turned out that large-scale simulations of the reference RVE can be replaced by simulating a combination of smaller solitary samples. This shortens the required simulation time and improves the memory usage of the simulation considerably, and thus substantially increases the efficiency of massive parallel computation for phase-field applications.

Shear-density coupling for a compressible single-component yield-stress fluid

M. Gross, F. Varnik
Soft Matter, **14**, 4577-4590 (2018)

Flow behavior of a single-component yield stress fluid is addressed on the hydrodynamic level. A basic ingredient of the model is a coupling between fluctuations of density and velocity gradient via a Herschel-Bulkley-type constitutive model. Focusing on the limit of low shear rates and high densities, the model approximates well - but is not limited to - gently sheared hard sphere colloidal glasses, where solvent effects are negligible. A detailed analysis of the linearized hydrodynamic equations for fluctuations and the resulting cubic dispersion relation reveals the existence of a range of densities and shear rates with growing flow heterogeneity. In this regime, after an initial transient, the velocity and density fields monotonically reach a spatially inhomogeneous stationary profile, where regions of high shear rate and low density coexist with regions of low shear rate and high density. The steady state is thus maintained by a competition between shear-induced enhancement of density inhomogeneities and relaxation via overdamped sound waves. An analysis of the mechanical equilibrium condition provides a criterion for the existence of steady state solutions. The dynamical evolution of the system is discussed in detail for various boundary conditions, imposing either a constant velocity, shear rate, or stress at the walls.

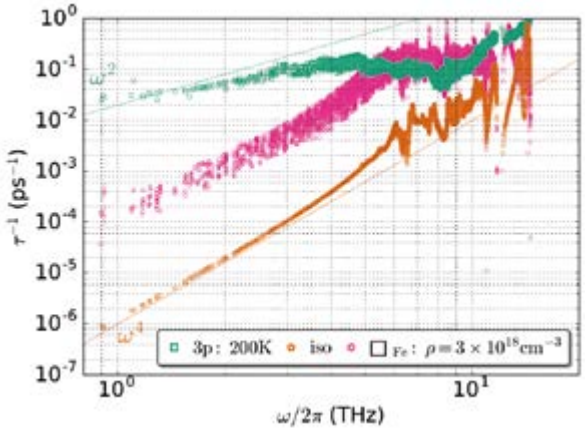


Growth direction and magnitude of the fluctuation amplitude of the most unstable mode. The coloring indicates the magnitude in a logarithmic scale, while the arrows indicate the growth direction (non-logarithmic scale along both axes), which is determined up to a sign. Accordingly, in the unstable region, fluctuations grow indefinitely by reducing the shear rate and increasing the density (or vice versa), providing a nonlinear feedback mechanism for the shear-density-coupling-instability.

Influence of point defects on the thermal conductivity in FeSi

R. Stern, T. Wang, J. Carrete, N. Mingo, G. Madsen
Physical Review B, **97**, 195201 (2018)

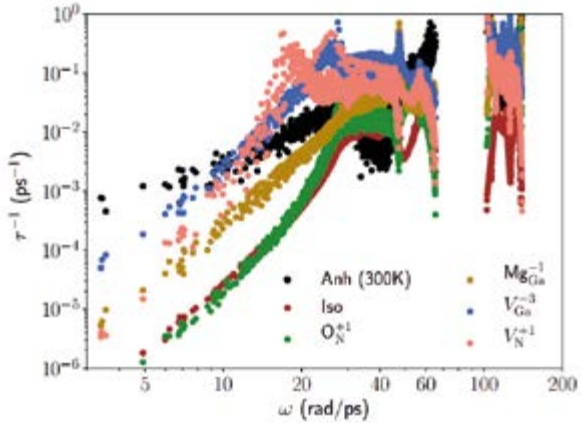
The unique transport properties of B20 FeSi have been investigated for decades. The progress in theoretical calculations allows the explanation and prediction of more and more of such properties. In this paper we investigate the lattice thermal conductivity of FeSi. Calculation for pristine FeSi severely overestimates the lattice thermal conductivity compared to experiment. We point out that the defect concentration can be considerably larger than indicated by the Hall coefficient. The defect formation energies are calculated and it is found that a substantial amount of iron vacancies can form at thermal equilibrium. These will lead to an increased phonon scattering. To explain the thermal conductivity of FeSi, we consider phonon-phonon, isotope, and phonon-defect scattering to assess possible scattering mechanisms. The calculated thermal conductivities indicate that phonon-defect scattering is important in order to explain the reported experimental values.



Multiple phonon scattering rates present in FeSi. For acoustic phonons with long wavelengths $1/\tau^{iso} \propto \omega^4$ for phonon-isotope scattering and $1/\tau^{\square Fe} \propto \omega^4$ for phonon-vacancy scattering.

Phonon transport unveils the prevalent point defects in GaN

A. Katre, J. Carrete, T. Wang, G. Madsen, N. Mingo
Physical Review Materials, **2**, 50602 (2018)



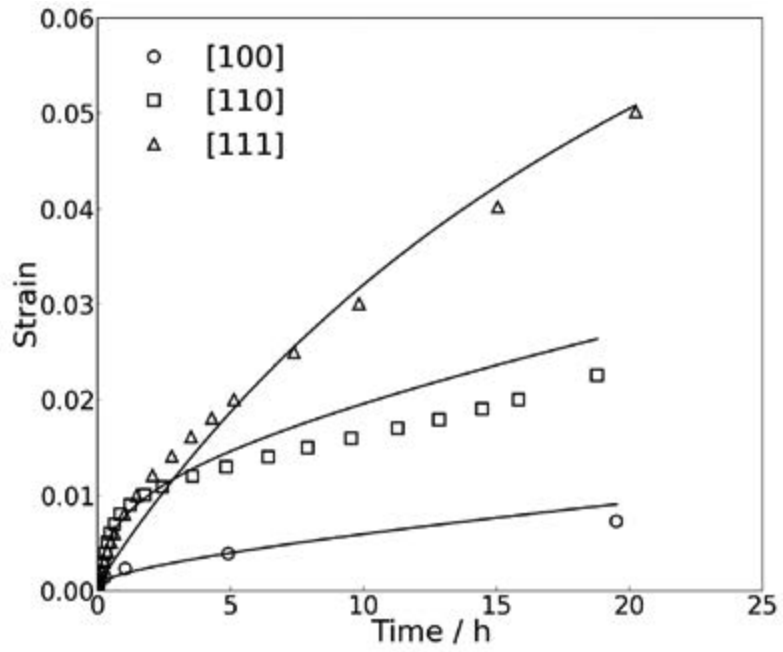
Phonon scattering rates (τ^{-1}) from different charged defects in GaN plotted with respect to phonon frequencies (ω). The defect concentration of 10^{20} cm^{-3} is considered here and the corresponding scattering rates are compared to anharmonic scattering at 300 K and isotope scattering. The corresponding defective GaN structures are also included in the SM.

Determining the types and concentrations of vacancies present in intentionally doped GaN is a notoriously difficult and long-debated problem. Here, we use an unconventional approach, based on thermal transport modeling, to determine the prevalence of vacancies in previous measurements. This allows us to provide conclusive evidence of the recent hypothesis that gallium vacancies in ammonothermally grown samples can be complexed with hydrogen. Our calculations for O-doped and Mg-O codoped samples yield a consistent picture interlinking dopant and vacancy concentration, carrier density, and thermal conductivity, in excellent agreement with experimental measurements. These results also highlight the predictive power of ab initio phonon transport modeling, and its value for understanding and quantifying defects in semiconductors.

A phenomenological creep model for nickelbase single crystal superalloys at intermediate temperatures

S. Gao, P. Wollgramm, G. Eggeler, A. Ma, A. Hartmaier, J. Scheuer
Modelling and Simulation in Materials Science and Engineering, **26**, 55001 (2018)

For the purpose of good reproduction and prediction of creep deformation of nickel-base single crystal superalloys at intermediate temperatures, a phenomenological creep model is developed, which accounts for the typical γ/γ′ microstructure and the individual thermally activated elementary deformation processes in different phases. The internal stresses from γ/γ′ lattice mismatch and deformation heterogeneity are introduced through an efficient method. The strain hardening, the Orowan stress, the softening effect due to dislocation climb along γ/γ′ interfaces and the formation of [112] dislocation ribbons, and the Kear-Wilsdorf-lock effect as key factors in the main flow rules are formulated properly. By taking the cube slip in [110]{100} slip systems and [112]{111} twinning mechanisms into account, the creep behavior for [110] and [111] loading directions are well captured. Without specific interaction and evolution of dislocations, the simulations of this model achieve a good agreement with experimental creep results and reproduce temperature, stress and crystallographic orientation dependences. It can also be used as the constitutive relation at material points in finite element calculations with complex boundary conditions in various components of superalloys to predict creep behavior and local stress distributions.



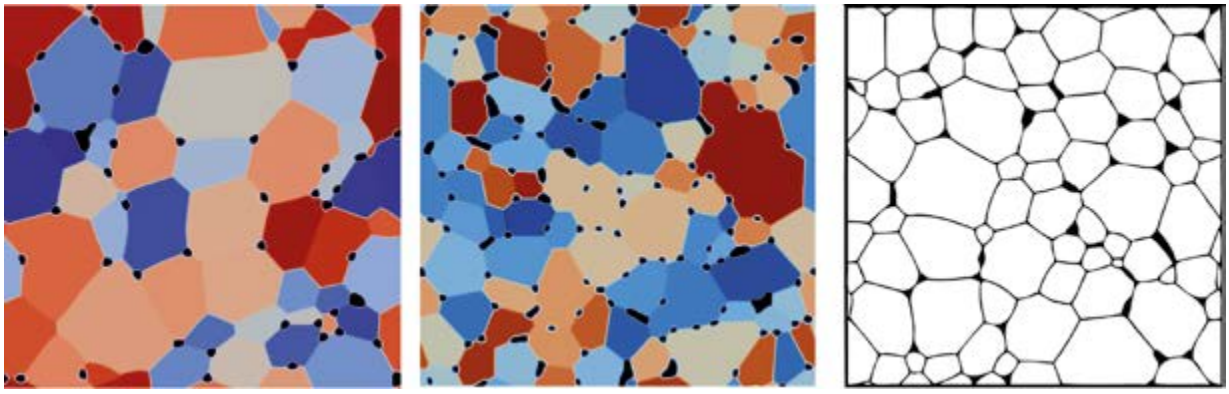
Comparison of simulation results and experimental data for creep curve undertensile load of 600 MPa at 850 Â°C for different directions; hollow symbols areexperimental data and solid lines are simulation results.

Phase-field modeling of pores and precipitates in polycrystalline system

J. Kundin, R. Schiedung, H. Sohaib, I. Steinbach
Modelling and Simulation in Materials Science and Engineering, **26**, 65003 (2018)

In this work, we develop an efficient phase-field approach to simulate the graingrowth in polycrystalline ceramic materials in the presence of pores withvarious mobilities and diffusion coefficients. The multi-phase-field model is coupled to the Cahn-Hilliard equation for pore dynamics by interaction functions which describe the interaction of pores with grain boundaries. Two types of the model are suggested with one and two order parameters responsible for the pores. We also show that the model can be applied to the simulation of the interaction of the grain boundaries with coherent and non-coherent particles. The parameters of the model allow us to reproduce the equilibrium dihedral angle in the triple-junction of a pore or a particle and a grain boundary. A drag velocity of the grain boundary in the presence of poresor precipitates was also measured for various diffusion coefficients and grain boundary mobilities. The effects of the pore dynamics on the grain size evolution in ceramic materials was investigated and compared with reported theoretical predictions and experimental data.

Simulated microstructure of grain growth with porosity for model type I and type II.

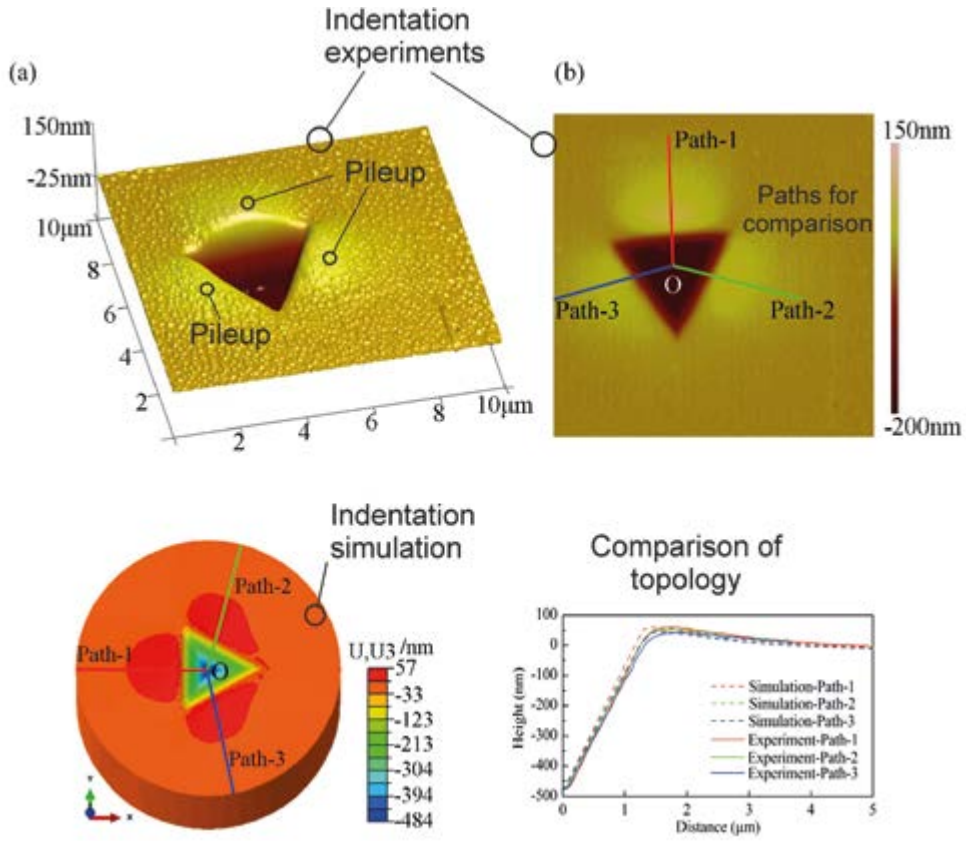


Coupled effect of crystallographic orientation and indenter geometry on nanoindentation of single crystalline copper

Z. Wang, J. Zhang, H. u. Hassan, J. Zhang, Y. Yan, A. Hartmaier, T. Sun
International Journal of Mechanical Sciences, **148**, 531-539 (2018)

Surface pile-up topography is very significant for property extraction in nanoindentation tests. In the present work, we perform crystal plasticity finite element simulations of Berkovich nanoindentation of single crystalline copper with different crystallographic orientations, which derive quantitatively comparable mechanical properties and surface pile-up topographies with experimental data. Simulation results demonstrate that there is acoupled effect of crystallographic orientation of indented material and indenter geometry on surface pile-up behavior, due to the interaction between intrinsic dislocation slip events and extrinsic discrete stress distribution patterns. Based on the relative spatial orientation between crystallographic orientation of indented material and indenter geometry, a surface pile-up density factor m p is proposed to qualitatively characterize the propensity of surface pile-up behavior in nanoindentation tests of single crystalline copper.

Experiment and simulation of nanoindentation and comparison of surface pileup topography.



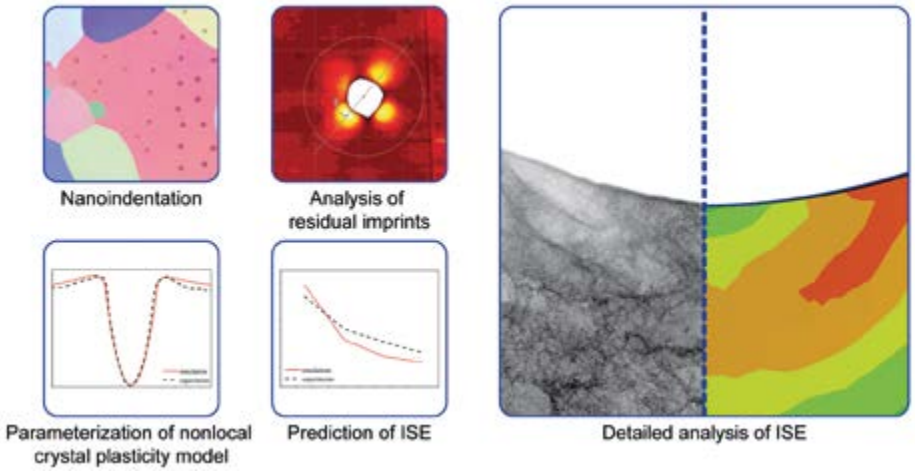
Indentation size effects in spherical nanoindentation analyzed by experiment and non-local crystal plasticity

J. K. Engels, S. Gao, W. Amin, A. Biswas, A. Kostka, N. Vajragupta, A. Hartmaier

Materialia, **3**, 21-30 (2018)

Nanoindentation has become a rather mature tool to characterize and measure mechanical properties of materials on micro- and nanometer length scales. However, the different types of indentation size effects (ISE) hamper the assessment of true, i.e., scale independent, material properties by nanoindentation. In the present study, the mechanisms of the ISE in spherical indentation have been investigated and quantified. Furthermore, it has been shown that the determination of non-local crystal plasticity parameters from nanoindentation results is possible. The thus-parameterized non-local crystal plasticity describes the higher-order size effect occurring in spherical indentation correctly and offers the possibility to understand the mutual contributions of geometrically necessary dislocations (GND) and statistically stored dislocations (SSD) to the material response. Nanoindentation experiments have been performed into a single grain of an ARMCO iron specimen, where the load displacement curves have been recorded, and the post-indentation surface topologies have been characterized. Furthermore, transmission electron microscopy has been performed to analyse the plastically deformed volume beneath the indentation. By comparing experimental and numerical nanoindentation results with respect to the plastic zone and dislocation structures, we validate the non-local crystal plasticity model of indentation and increase our understanding of the underlying mechanisms of the ISE in spherical indentation.

Experimental and numerical investigations on indentation size effects in spherical nanoindentation.

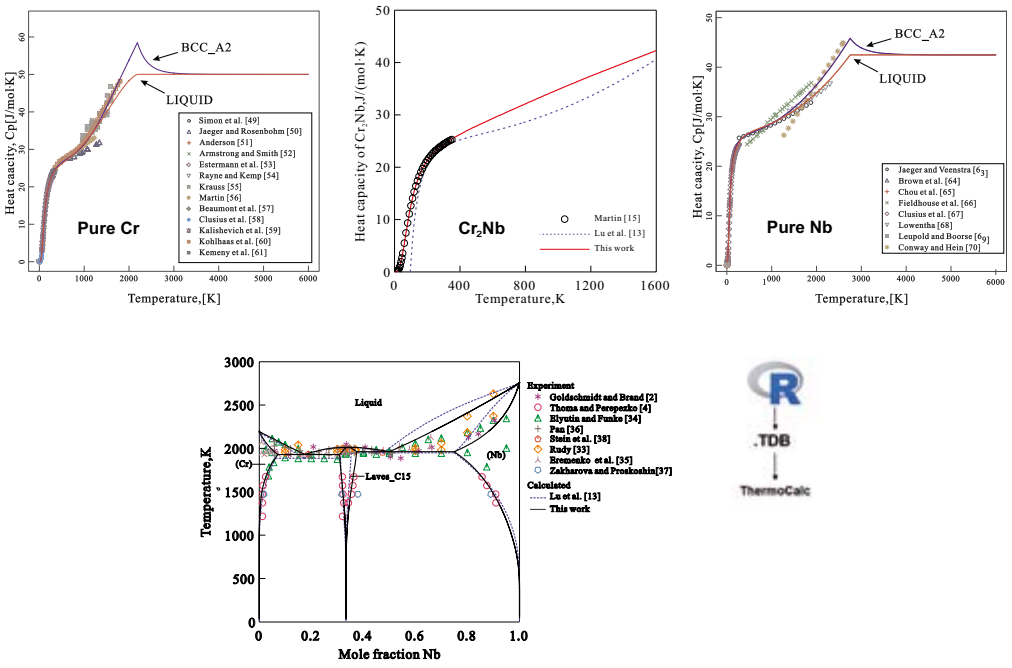


Thermodynamic re-assessment of binary Cr-Nb system down to 0 K

J. Yuxun, S. Zomorodpoosh, I. Roslyakova, L. Zhang
CALPHAD, **62**, 109-118 (2018)

Based on the recently proposed physically-based segmented model, the descriptions for Gibbs energy of pure Cr and Nb down to 0 K were first established. After that, a thermodynamic re-assessment of binary Cr-Nb system down to 0 K was then performed by taking into account all the experimental phase equilibria and thermodynamic properties. Especially, the experimental heat capacities of Cr_2Nb at low temperatures ignored in previous assessments were utilized in the present assessment. The calculated phase equilibria and thermodynamic properties according to the presently obtained thermodynamic descriptions of binary Cr-Nb system agree well with most of the experimental data, and show better agreement than the previous assessments.

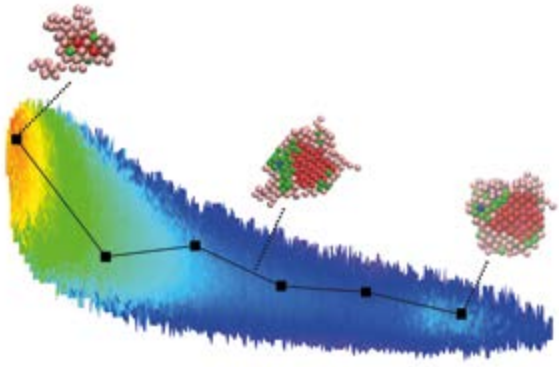
Results of thermodynamic re-assessment of binary Cr-Nb phase diagram from 0 K using segmented regression model. Upper graphs show obtained heat capacities for solid and liquid phases pure Cr, Nb and Cr_2Nb compound modeled by segmented regression model from 0 K.



Maximum likelihood analysis of reaction coordinates during solidification in Ni

G. Díaz Leines, J. Rogal
Journal of Physical Chemistry B, **122**, 10934-10942 (2018)

Understanding the underlying mechanism of crystal nucleation is a fundamental aspect in the prediction and control of materials properties. Classical nucleation theory (CNT) assumes that homogeneous nucleation occurs via random fluctuations within the supercooled liquid, that the structure of the growing clusters resembles the most stable bulk phase, and that the nucleus size is the sole reaction coordinate (RC) of the process. Many materials are, however, known to exhibit multiple steps during crystallization, forming different polymorphs. As a consequence, more complex RCs are often required to capture all relevant information about the process. Here, we employ transition path sampling together with a maximum likelihood analysis of candidate order parameters to identify suitable RCs for the nucleation mechanism during solidification in Ni. In contrast to CNT, the analysis of the reweighted path ensemble shows that a prestructured liquid region that surrounds the crystal cluster is a relevant order parameter that enhances the RC and therefore plays a key role in the description of the nucleus and the interfacial free energy. We demonstrate that prestructured liquid clusters that emerge within the liquid act as precursors of the crystallization in a nonclassical two-step mechanism, which predetermines the coordination of the selected polymorphs.

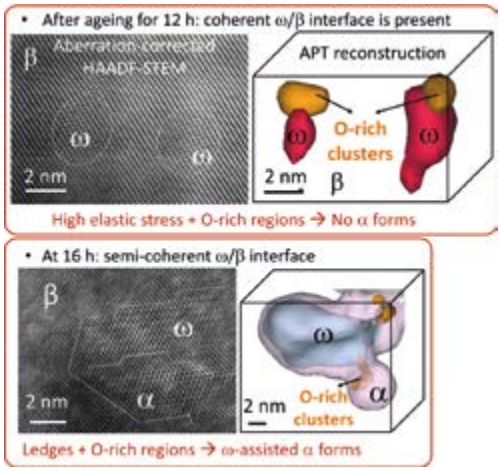


Optimal reaction coordinate (RC) and free energy landscape for nucleation during crystallization in nickel. The transition path on the free energy landscape evidences a two-step mechanism where an initial formation of a prestructured liquid region precedes the crystal nucleation and has a key role in the description of the RC.

Nucleation driving force for ω-assisted formation of α and associated ω morphology in β-Ti alloys

T. Li, D. Kent, G. Sha, H. Liu, S. G. Fries, A. V. Ceguerra, M. S. Darguschd, J. M. Cairney
Scripta Materialia, **155**, 149-154 (2018)

The structural and chemical changes at ω/β interfaces and the evolution of the morphology of ω in a near-β alloy during isothermal ageing at 573 K were investigated by atom probe tomography and aberration-corrected high-resolution transmission electron microscopy. Ledges and local O enrichment at semi-coherent isothermal ω interfaces are proposed to provide the key driving force for nucleation ω-assisted α. Following nucleation of α, the morphology of ω evolves from ellipsoidal to rod-like, induced by rapid consumption of ω by α.

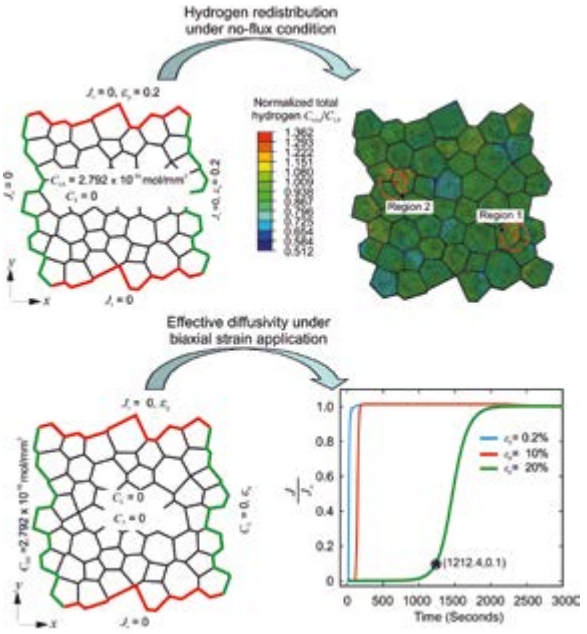


Structural and chemical changes at ω/β Ti alloys interfaces and the evolution of the morphology of ω in a near-β alloy at 12 and 16 hours isothermal ageing at 573 K.

Micromechanical modelling of coupled crystal plasticity and hydrogen diffusion

H. u. Hassan, K. Govind, A. Hartmaier
Philosophical Magazine, **99**, 92-115 (2018)

Hydrogen transport behaviour in metals is greatly influenced by the mechanical stress and the underlying microstructural features. In this work, a micromechanical model based on coupled crystal plasticity and hydrogen diffusion is developed and applied to model hydrogen diffusion and storage in a polycrystalline microstructure. Particular emphasis is laid on mechanical influences on hydrogen transport, invoked by internal stresses and by trapping of dislocations generated by plastic strains. First, a study of a precharged material is carried out where hydrogen is allowed to redistribute under the influence of mechanical loading. These simulations demonstrate to which extent hydrogen migrates from regions with compressive strains to those with tensile strains. In the next step, the influence of plastic prestraining on hydrogen diffusion is analysed. This prestraining produces internal residual stresses in the microstructure, that mimic residual stresses introduced into components during cold working. Lastly, a series of permeation simulations is performed to characterise the influence of hydrogen trapping on effective diffusivity. It is shown that the effective diffusivity decreases with stronger traps and the effect is more prominent at a larger predeformation, because the trapped hydrogen concentration increases considerably. The reduction of effective diffusivity with plastic deformation agrees very well with experimental findings and offers a way to validate and parameterise our model. With this work, it is demonstrated how micromechanical modelling can support the understanding of hydrogen transport on the microstructural level.



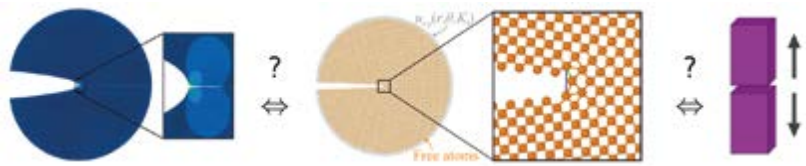
Numerical modeling of the hydrogen distribution in the microstructure under no-flux boundary condition (top image) and the influence of biaxial strain on the effective diffusivity (bottom image). Initial and boundary conditions are given on the left side and results on the right side.

Fracture ab initio: A force-based scaling law for atomistically informed continuum models

J. Möller, E. Bitzek, R. Janisch, H. ul Hassan, A. Hartmaier
Journal of Materials Research, **33**, 3750-3761 (2018)

In fracture mechanics, established methods exist to model the stability of a crack tip or the kinetics of crack growth on both the atomic and the macroscopic scales. However, approaches to bridge the two scales still face the challenge in terms of directly converting the atomic forces at which bonds break into meaningful continuum mechanical failure stresses. Here we use two atomistic methods to investigate cleavage fracture of brittle materials: (i) we analyze the forces in front of a sharp crack and (ii) we study the bond breaking process during rigid body separation of half crystals without elastic relaxation. The comparison demonstrates the ability of the latter scheme, which is often used in ab initio density functional theory calculations, to model the bonding situation at a crack tip. Furthermore, we confirm the applicability of linear

elastic fracture mechanics in the nanometer range close to crack tips in brittle materials. Based on these observations, a fracture mechanics model is developed to scale the critical atomic forces for bond breaking into relevant continuum mechanical quantities in the form of an atomistically informed scale-sensitive traction separation law. Such failure criteria can then be applied to describe fracture processes on larger length scales, e.g., in cohesive zone models or extended finite element models.



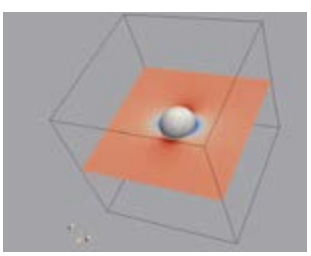
A novel approach to bridge the scales from atoms to continuum in fracture modeling has been developed. With a physically consistent scaling law, data from density-functional calculations of atomic bond characteristics (right subfigure) can be directly applied in continuum fracture models (left subfigure). The approach has been validated with molecular dynamics simulations (middle subfigure), see Möller et al., JMR 33 (2018) 3750; https://doi.org/10.1557/jmr.2018.384.

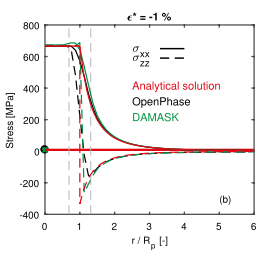
Numerical benchmark of phase-field simulations with elastic strains: Precipitation in the presence of chemo-mechanical coupling

R. Darvishi Kamachali, C. Schwarze, M. Lin, M. Diehl , P. Shanthraj, U. Prahl, I. Steinbach, D. Raabe
Computational Materials Science, **155**, 541-553 (2018)

Phase-field studies of solid-state precipitation under strong chemo-mechanical coupling are performed and benchmarked against the existing analytical solutions. The open source software packages OpenPhase and DAMASK are used for the numerical studies. Solutions for chemical diffusion and static mechanical equilibrium are investigated individually followed by a chemo-mechanical coupling effect arising due to composition dependence of the elastic constants. The accuracy of the numerical solutions versus the analytical solutions is quantitatively discussed. For the chemical diffusion benchmark, an excellent match, with a deviation <0.1%, was obtained. For the static mechanical equilibrium benchmark Eshelby problem was considered where a deviation of 5% was observed in the normal component of the stress, while the results from the diffuse interface (OpenPhase) and sharp interface (DAMASK) models were slightly different. In the presence of the chemo-mechanical coupling, the concentration field around a static precipitate was benchmarked for different coupling coefficients. In this case, it is found that the deviation increases proportional to the coupling coefficient that represents the strength of coupling concentration and elastic constants. Finally, the interface kinetics in the presence of the considered chemo-mechanical coupling were studied using OpenPhase and a hybrid OpenPhase–DAMASK implementation, replacing the mechanical solver of OpenPhase with DAMASK's. The observed deviations in the benchmark studies are discussed to provide guidance for the use of these results in studying further phase transformation models and implementations involving diffusion, elasticity and chemo-mechanical coupling effect.

Stress distribution in the Eshelby benchmark test against the analytical solution with different softwares. Left: Stress distribution perpendicular to the cross section in colour. Right: Normal and tangential stress in radial direction.





ICAMS

ICAMS Members 2017 and 2018

13. ICAMS Members 2017 and 2018

Staff at ICAMS

About 73 researchers, including PhD students, work at ICAMS; about 5 administrative staff and 3 technicians support the institute.

Figure 13.1 shows the development of ICAMS staff numbers through the past ten years. By the end of 2008 about 30 people were working at ICAMS. From 2009 to 2014 this number increased and by the end of 2014 almost 90 people worked at ICAMS. In 2016 ICAMS' staff numbers have decreased to the level of 2012 but in 2017 and 2018 the number increased again to almost 81 people.

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

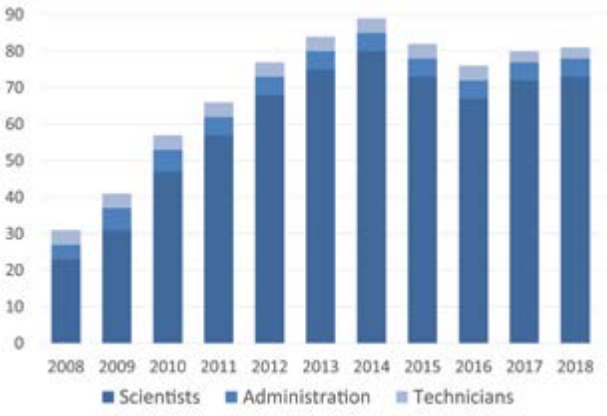


Fig. 13.1: Development of ICAMS staff from 2008 to 2018.

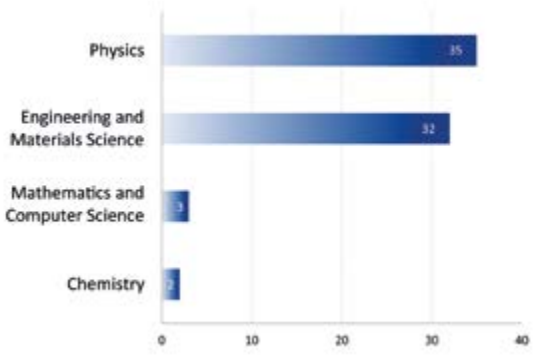
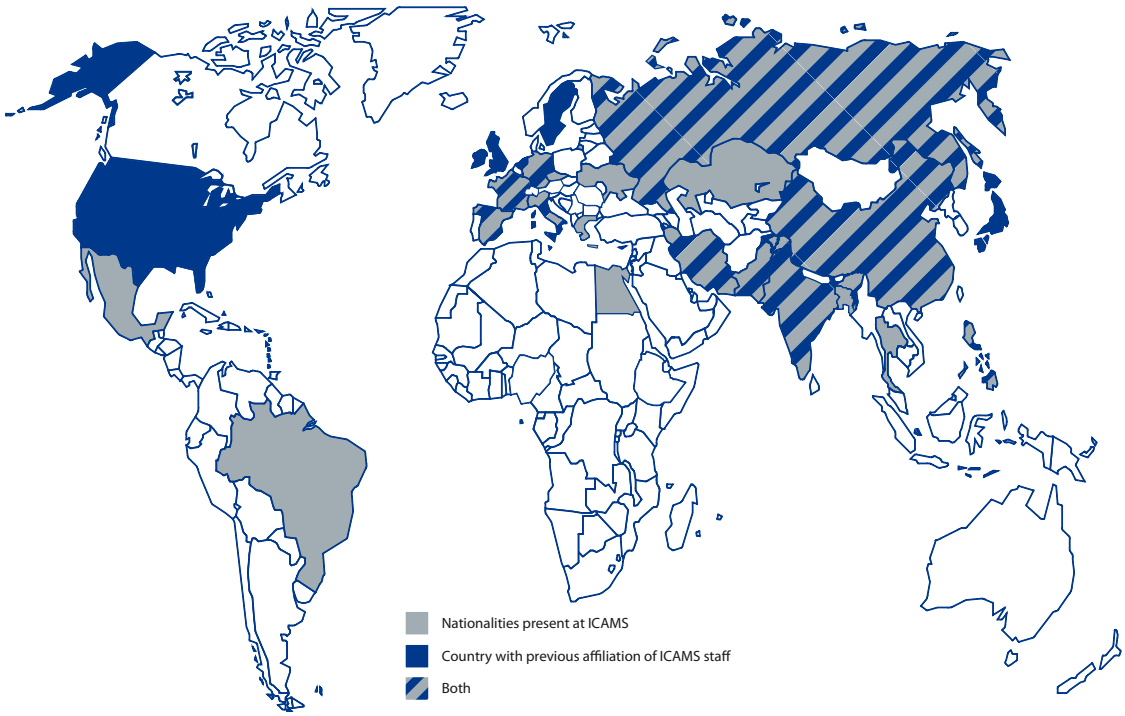


Fig. 13.2: Breakdown of first degree of ICAMS researchers in 2017/2018.

In 2017 and 2018 researchers from 19 different countries were working at ICAMS (see grey areas in *Figure 13.3*). 44% of the ICAMS staff is of German and 56% of foreign nationality. For ICAMS, it is of vital importance to attract talented scientists from leading research institutions worldwide.

Figure 13.3 gives an overview of the countries and institutions of origin of the current ICAMS researchers. 13 of the 41 institutions are located in Germany, 12 in other EU countries and 16 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

China
Beihang University, Beijing
Harbin Institute of Technology, Harbin
Tianjin University, Tianjin
Northwestern Polytechnical Univ., Xi'an Shaanxi

France
LEM-ONERA-CNRS, Chatillion
CNRS, Paris

Germany
AICE, Aachen
RWTH Aachen
Universität Bayreuth
Ruhr-Universität Bochum
TU Dortmund
MPI für Eisenforschung, Düsseldorf
Friedrich-Alexander Univ., Erlangen-Nürnberg
Universität Duisburg-Essen
Fraunhofer IWM, Freiburg
FH Gelsenkirchen
Georg-August Universität Göttingen
Universität Heidelberg
BASF, Ludwigshafen

India
Indian Institute of Technology, Bombay
Indian Institute of Technology, Guwahati
JNTU Heiderabad
Indian Institute of Science, Karnataka

Iran
University of Guilan, Rasht
Sahand University of Technology
Shiraz University
Amirkabir University of Technology, Teheran

Ireland
Trinity College, Dublin

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

Japan
University of Tokio

The Netherlands
University of Amsterdam

Pakistan
Ghulam Ishaq Khan Institute of Engineering

Philippines
De La Salle University, Manila

Russia
Kazan Federal University
JIHT Moskow

Spain
University of la Coruna

Sweden
University of Linköping

United Kingdom
University of Oxford

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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ICAMS

Publications

14. Publications

W. Ko, S. Maisel, B. Grabowski, J. Jeon, J. Neugebauer
Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys
Acta Materialia, 123, 2017, 90-101

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Zeitschrift fur Naturforschung A, 72, 2017, 51-58

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Solid State Phenomena, 258, 2017, 43741

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almaBTE: A solver of the space-time dependent Boltzmann transport equation for phonons in structured materials
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Effects of incident N atom kinetic energy on TiN/TiN(001) film growth dynamics: A molecular dynamics investigation
Journal of Applied Physics, 121, 2017, 25302

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Journal of Physics: Condensed Matter, 29, 2017, 95501

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Acta Materialia, 124, 2017, 305-315

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Materials Science and Engineering A, 685, 2017, 19-30

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Journal of Alloys and Compounds, 693, 2017, 1315-1322

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J. V. Görler, I. Lopez-Galilea, L. Mujica, O. Shchyglo, W. Theisen, I. Steinbach
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Acta Materialia, 124, 2017, 151-158

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Physical Review B, 95, 2017, 104108

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Physical Review B, 95, 2017, 94307

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Journal of the Mechanics and Physics of Solids, 102, 2017, 209-223

A. Hartmaier
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Implementation of an effective bond energy formalism in the multicomponent Calphad approach
Journal of Research of National Institute of Standards and Technology, 123, 2018, 123020

J. Möller, E. Bitzek, R. Janisch, H. ul Hassan, A. Hartmaier
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A. G. Kiiamov, Y. Lysogorskiy, F. G. Vagizov, L. R. Tagirov, D. A. Tayurskii, Z. Seidov, H.-A. Krug von Nidda, V. Tsurkan, D. Croitori, A. Günther, F. Mayr, A. Loidl
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Physical Review B, 98, 2018, 214411

S. Gupta, A. Ma, A. Hartmaier
Mechanical twinning induced alteration in the kinetics of martensitic phase transformation in TRIP-maraging steels
International Journal of Solids and Structures, 155, 2018, 213-224

X. Zhang, B. Grabowski, F. Körmann, A. V. Ruban, Y. Gong, R. C. Reed, T. Hickel, J. Neugebauer
Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni
Physical Review B, 98, 2018, 224106

S. Katnagallu, B. Gault, B. Grabowski, J. Neugebauer, D. Raabe, A. Nematollahi
Advanced data mining in field ion microscopy
Materials Characterization, 146, 2018, 307-318

M. Vaidya, G. M. Muralikrishna, S. V. Divinski, B. S. Murty
Experimental assessment of the thermodynamic factor for diffusion in CoCrFeNi and CoCrFeMnNi high-entropy alloys
Scripta Materialia, 157, 2018, 81-85

R. Darvishi Kamachali, C. Schwarze, M. Lin, M. Diehl, P. Shanthraj, U. Prahl, I. Steinbach, D. Raabe
Numerical benchmark of phase-field simulations with elastic strains: Precipitation in the presence of chemo-mechanical coupling
Computational Materials Science, 155, 2018, 541-553

H. Ganesan, C. Teijeiro Barjas, G. Sutmann
Parallelization comparison and optimization of a scale-bridging framework to model Cottrell atmospheres
Computational Materials Science, 155, 2018, 439-449

ICAMS

Talks and Posters

15. Talks and Posters

13.01.2017
J. Rogal
Atomistic mechanisms and kinetics during phase transformations in metals
18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy

16.01.2017
T. Hickel, E. J. McEniry, P. Dey, J. Neugebauer, M. Mrovec, D. Di Stefano, C. Elsässer
The first principles approach: Insights into hydrogen trapping by microstructures in steels
Royal Society Discussion Meeting: The challenges of hydrogen and metals, London, UK

17.01.2017
J. Rogal
A kinetic Monte Carlo approach to diffusion controlled thermal desorption spectroscopy
Royal Society Discussion Meeting: The challenges of hydrogen and metals, London, UK

16.02.2017
F. Varnik
Shear localization in amorphous solids: The role of structure and long range spatio-temporal correlations of fluctuations
Bridging the Scales in Glasses II, University of Mainz, Germany

21.02.2017
I. Steinbach
Atomistically informed full-field simulation of applied materials: Aspects of thermo-chemo-mechanical coupling
CDMSI International Workshop on scale bridging for the atomistic design of high performance materials, Tokyo, Japan

26.02.2017
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Ab Initio guided design of high strength steels: Where do we stand?
TMS Annual Meeting, San Diego, USA

26.02.2017
F. Körmann, I. Bleskov, B. Grabowski, B. Dutta, T. Hickel, J. Neugebauer
Parameter-free finite-temperature computations of stacking fault energies for magnetic materials
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28.02.2017
M. Mrovec, D. Di Stefano, C. Elsässer, R. Nazarov, T. Hickel, J. Neugebauer
New insights into H trapping and diffusion in steel microstructures obtained from atomistic simulations
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13.03.2017
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Ab initio guided design of structural materials with superior mechanical properties
APS Meeting 2017, New Orleans, USA

05.04.2017
J. Neugebauer
How to achieve interoperability – A modeler's perspective
1st EMMC International Workshop, Vienna, Austria

03.05.2017
R. Janisch, X. Pang, M. Kanani, A. Izardar, A. Hartmaier
Grain boundary properties:
Insights from atomistic simulations and their use in mechanical modeling of materials
SFB 986 Materials Science Colloquium, Technical University Hamburg, Germany

05.05.2017
J. Neugebauer
From semiconductors to high-strength steels and back again
10 years of the Laboratory for Photovoltaics & Semiconductor Physics, Luxembourg

17.05.2017
R. Drautz
Density functional theory in a nutshell
Doctoral Retreat of SFB 1242, Hamminkeln, Germany

22.05.2017
A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer, M. Leitner, J. Neuhaus, W. Petry
Ab initio determination of phonon lifetimes up to the melting point
EMRS Spring Meeting 2017, Strasbourg, France

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Atomistic origins of deformation at grain boundaries in Al and TiAl
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Machine learning as tool to enhance ab initio based alloy design
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Atomistically informed full-field simulation of quenching, tempering and testing of martensitic steel
Ostbayerische Technische Hochschule Regensburg, Germany

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R. Janisch, M. Kanani, X. Pang, A. M. Tahir, A. Hartmaier
Deformation and fracture at grain boundaries: Can we include atomistic effects in mesoscale descriptions via a few physical parameters?
14th International Conference on Fracture, Ixia, Greece

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M. Todorova, A. K. Vatti, S. Yoo, J. Neugebauer
Ab initio modelling of electrochemical processes: Challenges and insights
Fundamental Electrochemistry: Theory Meets Experiment, Lorentz Center, Leiden, Netherlands

28.06.2017
M. Mrovec
Atomistic simulations of mechanical behavior using bond order potentials
Université de Lille, France

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R. Drautz
From electrons to properties of materials
Colloquium Materials Modelling, IMWF, Stuttgart, Germany

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From density functional theory to analytic magnetic bond-order potentials
Warwick EPSRC Symposium:
Density functional theory and beyond: Analysis and computation, Coventry, UK

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B. Grabowski
Data driven engineering of advanced materials: Combining high precision and scale bridging
Forschungszentrum Jülich, Germany

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Why solidification? Why phase-field?
6th Decennial International Conference on Solidification Processing, Old Windsor, UK

22.08.2017
J. Rogal
Finding reaction coordinates during phase transformations in metals
53rd Symposium on Theoretical Chemistry, Basel, Switzerland

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A. Hartmaier
Atomistically informed continuum models for deformation and fracture of materials
International Symposium on Multiscale Computational Analysis of Complex Materials, Copenhagen, Denmark

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H. u. Hassan, M. Boeff, A. Hartmaier
Modelling and experiment of material-oriented micro/nano manufacturing
Sino-German Symposium: Modeling and Experiment of Material-oriented Micro/Nano Manufacturing, Harbin, China

11.09.2017
T. Hickel, I. Bleskov, U. Aydin, F. Körmann, B. Grabowski, J. Neugebauer
Quantum mechanically guided materials design
Summer school: Materials 4.0 – The digitally enabled atom to system revolution, Dresden, Germany

12.09.2017
T. Hammerschmidt
Prediction of alloying windows and alloying routes with a 3D structure map
Big-Data driven Materials Science Workshop, Lausanne, Switzerland

14.09.2017
J. Rogal
Atomistic mechanisms and kinetics during phase transformations in metals
Psi-k Workshop on Theory and Simulation Challenges of Nano Phase-Change Materials, Coventry, UK

19.09.2017
H. u. Hassan, W. Ye, A. Hartmaier
Micromechanical modeling of fatigue crack initiation in aluminium 2024
EUROMAT 2017, Thessaloniki, Greece

20.09.2017
I. Steinbach
Atomistically informed full-field simulation of tempered martensite: Quenching, tempering and mechanical characterization
EUROMAT 2017, Thessaloniki, Greece

20.09.2017
R. Drautz
From density functional theory to analytic magnetic bond-order potentials and the calculation of thermodynamic properties
EUROMAT 2017, Thessaloniki, Greece

22.09.2017
J. Neugebauer, T. Hickel
Modelling structural materials in realistic environments by ab initio thermodynamics
EUROMAT 2017, Thessaloniki, Greece

08.10.2017
B. Grabowski, C. Race, J. Neugebauer
Atomistic simulations on grain boundary migration
MS&T, Pittsburgh, USA

09.10.2017
J. Neugebauer, T. Hickel, Z. Pei, J. Janßen
Materials discovery and design at finite temperatures
MS&T, Pittsburgh, USA

11.10.2017
S. Münstermann, B. Döbereiner, D. Novokshanov
Design of damage tolerance in high-strength steels
MPA-Seminar, Stuttgart, Germany

16.10.2017
M. Todorova, A. K. Vatti, S. Yoo, J. Neugebauer
Free energy sampling for electrochemical systems
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA, USA

16.10.2017
J. Neugebauer
Free energy sampling strategies for structurally complex materials
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA, USA

16.10.2017
J. Neugebauer
Stochastic sampling and accelerated time dynamics on multidimensional surfaces
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA, USA

17.10.2017
J. Rogal
Finding reaction coordinates for phase transformations in metals
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA, USA

06.11.2017
M. Mrovec
Atomistic simulations of extended defects using coarse-grained electronic structure methods
Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

14.11.2017
I. Stockem
The interaction of spin dynamics and lattice vibrations of CrN in the paramagnetic state
BIfAM Seminar, Bielefeld, Germany

21.11.2017
B. Dutta, F. Körmann, J. Neugebauer, T. Hickel
Temperature-driven effects in functional materials: Ab initio insights
Université Pierre and Marie Curie, Paris, France

28.11.2017
J. Rogal
Finding reaction coordinates during phase transformations in solids
MRS Fall Meeting, Boston, USA

04.12.2017
B. Grabowski
Knowledge driven engineering of metals: Development and application of ab initio based scale bridging methods
TU Delft, Netherlands

10.01.2018
A. Glensk
From thermodynamics to phonon lifetimes: Anharmonic calculations with ab initio accuracy
CECAM workshop: Anharmonicity and thermal properties of solids, Paris, France

31.01.2018
R. Drautz
From the atomic interaction to thermodynamic and mechanical properties of materials
Physikalisches Kolloquium, TU Chemnitz, Germany

02.02.2018
J. Rogal
Atomistic insight into the dynamics and mechanisms of phase transformations in metals
Penn Institute for Computational Science Colloquium, Philadelphia, USA

08.02.2018
I. Steinbach
Why Phase-field?
5th GAMM Workshop on Phase-field Modelling, TU Dresden, Germany

09.02.2018
J. Rogal
Atomistic insight into the dynamics and mechanisms of phase transformations in materials
NYU Chemistry Seminar, New York University, USA

15. 02. 2018
B. Dutta, F. Körmann, T. Hickel, J. Neugebauer
Role of temperature dependent excitations and the coupling between them in functional materials: Ab initio insights
Linköping University, Sweden

15. 02. 2018
P. Dey, T. Hickel, J. Neugebauer
Understanding hydrogen embrittlement based on ab initio methods
Linköping University, Sweden

23. 02. 2018
S. G. Fries
Magnetic degrees of freedom, state of the art first-principles/CALPHAD modeling approaches
IMR Seminar, Tohoku University, Sendai, Japan

26. 02. 2018
T. Hickel, I. Bleskov, P. Dey, F. Körmann,
B. Grabowski, J. Neugebauer
Strengthening mechanisms in a precipitation hardened high-Mn lightweight steel
6th ESISM Workshop on Fundamental Issues of Structural Materials, Kyoto, Japan

26. 02. 2018
J. Neugebauer, M. Todorova, B. Grabowski,
T. Hickel, G. P. Leyson
Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach
Max-Planck-Institut für Plasmaphysik, Garching, Germany

26. 02. 2018
B. Grabowski, S. Hadian, A. Nematollahi, C. Kirchlechner,
G. Dehm, J. Neugebauer, W. Ko, J. B. Jeon
Dislocation twin boundary interactions in nanoscale Cu bi-crystals: Simulation versus experiment
Schöntal Symposium – Dislocation based Plasticity, Schöntal, Germany

07. 03. 2018
I. Steinbach
Multi-scale simulation of Ni-base turbine blades: From solidification to rafting under creep conditions
Industrial Colloquium of the SFB/TR103, Fürth, Germany

11. 03. 2018
J. Neugebauer, J. Janßen, F. Körmann,
B. Grabowski, T. Hickel
Exploration of large ab initio data spaces to design structural materials with superior mechanical properties
Hume-Rothery Award Symposium, TMS Conference, Phoenix, USA

11. 03. 2018
T. Hickel, J. Neugebauer, F. Körmann,
B. Grabowski, M. Todorova
Modelling structural materials in realistic environments by ab initio thermodynamics
TMS conference, Phoenix, USA

12. 03. 2018
B. Grabowski, J. Neugebauer
Efficient and accurate computation of melting temperatures and enthalpies and entropies of fusion from ab initio
TMS conference, Phoenix, USA

26. 03. 2018
S. G. Fries
Magnetic degrees of freedom, state of the art first-principles/CALPHAD modeling approaches
Laboratory of Semiconductor Materials, EPFL, Lausanne, Switzerland

29. 03. 2018
I. Steinbach
Why Phase-field?
Hong Kong University of Science and Technology, Hong Kong, China

29. 03. 2018
J. Rogal
Interstitial and substitutional diffusion in metals
International Seminar series on Time Dependent Multiscale Phenomena of Materials Tohoku University, Sendai, Japan

29.03.2018
M. Grabowski, J. Rogal, R. Drautz
Modelling diffusion in non-dilute Ni-Re alloys: A combined kinetic Monte Carlo and cluster expansion approach
International Seminar series on Time Dependent Multiscale Phenomena of Materials, Tohoku University, Sendai, Japan

29.03.2018
M. Mrovec
Atomistic simulations of extended defects using coarse-grained electronic structure methods
Masaryk University, Brno, Czech Republic

03.04.2018
J. Neugebauer, L. Zhu, F. Körmann, B. Grabowski, T. Hickel
From electrons to the design of structurally complex materials
SFB ViCoM conference EPT 2018: From electrons to phase transitions, Vienna, Austria

10.04.2018
M. Todorova, S. Surendralal, S. Yoo, J. Neugebauer
Atomistic insights into surface stability and reactivity at solid/liquid interfaces from first principles calculations
Technical University Vienna, Austria

16.04.2018
T. Hickel, A. Glensk, R. Nazarov, U. Aydin, B. Grabowski, O. Hedge, J. Neugebauer
Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction
2018 Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments, Trieste, Italy

23.04.2018
R. Drautz
From the atomic interaction to thermodynamic and mechanical properties of materials
45th International Conference on Metallurgical Coatings and Thin Films, San Diego, USA

24.04.2018
I. Roslyakova, S. Zomorodpoosh, A. Obaied, Y. Jiang, L. Zhang, R. Otis, B. Bocklund
Third generation CALPHAD databases by automated statistical regression analysis
HERO-M Seminar, KTH Royal Institute of Technology, Stockholm, Sweden

25.04.2018
I. Roslyakova, I. Steinbach
Property models for Ni-based superalloys: Physically-based and statistical modelling approaches
Thermo Calc Software AB, Solna, Sweden

18.05.2018
B. Grabowski
Knowledge driven engineering of materials: Development and application of ab initio based scale bridging methods
Helmut-Schmidt-Universität Hamburg, Germany

01.06.2018
T. Hickel
Characterizing complex materials by ab initio methods
Abteilungskolloquium, BAM Berlin, Germany

14.06.2018
R. Drautz
From electrons to interatomic interactions and to properties of materials
Kolloquium SFB 716, Universität Stuttgart, Germany

14.06.2018
T. Hickel, B. Grabowski, F. Körmann, A. Glensk
Understanding phase stabilities and microstructure formation with finite temperature ab initio methods
MPIE Lecture Series, Düsseldorf, Germany

04.07.2018
T. Hammerschmidt, M. Čák, J. Jenke, A. C. Ladines, Y. Lysogorskiy, A. P. Subramanyam, N. Wang, R. Drautz
Parameterisation and transferability of analytic bond-order potentials
Modern Approaches to Coupling Scales In Materials Simulations Workshop, Lenggries, Germany

04. 07. 2018
S. G. Fries
High temperature, high expectations
XVI International IUPAC conference on high temperature materials chemistry (HTMC-XVI), Ekaterinburg, Russia

08. 07. 2018
O. Waseda
Machine-learning assisted Heisenberg model for systems with ill-defined magnetic interactions
Thermec 2018 Conference, Paris, France

10. 07. 2018
T. Hickel, P. Dey, B. Dutta, M. Friák, J. Neugebauer
Phase stability and chemical composition of nano precipitates: A first principles study for the example of κ carbides
Thermec 2018 Conference, Paris, France

11. 07. 2018
J. Neugebauer, S. Hadian, L. Huber, C. Race, B. Grabowski
Modelling thermodynamics and kinetics of general grain boundaries: Challenges and successes
Thermec 2018 Conference, Paris, France

11. 07. 2018
R. Drautz
Analytic bond-order potentials for transition metals
David Pettifor Scientific Symposium, Oxford, UK

11. 07. 2018
M. Mrovec
Atomistic simulations of extended defects using bond-order potentials
David Pettifor Scientific Symposium, Oxford, UK

11. 07. 2018
T. Hammerschmidt, B. Seiser, A. Bialon, J. Koßmann, J. Jenke, A. P. Subramanyam, Y. Lysogorskiy, D. G. Pettifor, R. Drautz
Prediction of structural stability with structure maps
David Pettifor Scientific Symposium, Oxford, UK

12. 07. 2018
I. Steinbach
Phase-field and CALPHAD
2018 SIAM Conference on Mathematical Aspects of Material Science, Portland, USA

12. 07. 2018
I. Roslyakova, I. Steinbach
Third generation CALPHAD databases by automated statistical regression analysis
2018 SIAM Conference on Mathematical Aspects of Material Science, Portland, USA

19. 07. 2018
J. Rogal
Extended timescale simulations of atomistic processes during phase transformations in materials
CRC 1114 – Colloquium, FU Berlin, Germany

03. 09. 2018
T. Hammerschmidt, B. Seiser, A. Bialon, J. Koßmann, D. G. Pettifor CBE FRS, R. Drautz
Navigating chemical compound space with structure maps
Materials Discovery Symposium, Liverpool, UK

09. 09. 2018
M. Mrovec
Atomistic studies of dislocations in iron using magnetic bond-order potential
Multiscale Modelling of Materials for Sustainable Development Conference, Vietnam National University, Hanoi, Vietnam

13. 09. 2018
A. Hartmaier
What does nanoindentation teach us on macroscopic material behavior
Indentation 2018, Liège, Belgium

26. 09. 2018
Y. Lysogorskiy
Locally approximated electronic structure based descriptors for predicting materials properties
A hands-on course on tools for novel-materials discovery, Lausanne, Switzerland

01. 10. 2018
J. Rogal
Analysis of reaction coordinates for nucleation in metals
E-CAM State-of-the Art Workshop: Large Scale Activated Event Simulations, Vienna, Austria

10.10.2018
T. Hammerschmidt
Analytic bond-order potentials: From downfolding DFT eigenspectra to large-scale atomistic simulations
Frontiers in Molecular Dynamics: Machine Learning, Deep Learning and Coarse Graining Workshop, Tel-Aviv, Israel

12.10.2018
I. Steinbach, M. A. Ali, J. V. Görler
Full-field simulation of Ni-base turbine blades: From precipitation to rafting and under creep conditions
Society of Engineering Sciences 2018, Madrid, Spain

15.10.2018
J. Neugebauer, L. Zhu, F. Körmann, B. Grabowski, T. Hickel
Data driven approaches in materials design: Theory meets experiment
RCTP-2018 Conference, Moscow, Russia

18.10.2018
S. G. Fries, U. R. Kattner
Effective bond energy formalism in the multi-component CALPHAD approach: An improvement of TCP phases descriptions based on first-principles data
Hero-m 2i, KTH, Stockholm, Sweden

26.10.2018
J. V. Görler, M. A. Ali, O. Shchyglo, I. Steinbach
Simulation of rafting and topological inversion in Ni-base superalloys
2018 KIM Fall Conference: Symposium on Microstructure Modeling of Materials, Daejeon, South Korea

26.10.2018
I. Steinbach, M. A. Ali, O. Shchyglo, C. Koerner
Stress-strain evolution during rapid solidification and self-tempering of additive manufactured Ni-base superalloys simulated by a mesoscopic phase-field model
2018 KIM Fall Conference: Symposium on Microstructure Modeling of Materials, Daejeon, South Korea

28.10.2018
J. Neugebauer, J. Janßen, F. Körmann, B. Grabowski, T. Hickel
Exploration of large ab initio data spaces to design structural materials with superior mechanical properties
9th International Conference on Multiscale Materials Modeling, Osaka, Japan

30.10.2018
M. Todorova, S. Yoo, S. Surendralal, J. Neugebauer
Ab initio modelling of solid/liquid interfaces: Challenges and insights
FS Seminar, DESY, Hamburg, Germany

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Atomistic processes at interfaces on extended timescales
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08.11.2018
J. Neugebauer
Electronic structure and computational metallurgy
EMMC Expert meeting and roadmap, CECAM-HQ-EPFL, Lausanne, Switzerland

21.11.2018
R. Drautz
From electrons to properties of materials
8th NRW Nano Conference, Dortmund, Germany

ICAMS

Seminars and other Lectures

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From semiconductors to high-strength steels and back again
10 years of the Laboratory for Photovoltaics & Semiconductor Physics, Luxembourg

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Ab initio modelling of electrochemical processes: Challenges and insights
Fundamental Electrochemistry: Theory Meets Experiment, Lorentz Center, Leiden, Netherlands

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H. u. Hassan, M. Boeff, A. Hartmaier
Modelling and experiment of material-oriented micro/nano manufacturing
Sino-German Symposium: Modeling and Experiment of Material-oriented Micro/Nano Manufacturing, Harbin, China

11.09.2017
T. Hickel, I. Bleskov, U. Aydin, F. Körmann, B. Grabowski, J. Neugebauer
Quantum mechanically guided materials design
Summer school: Materials 4.0 – The digitally enabled atom to system revolution, Dresden, Germany

12.09.2017
T. Hammerschmidt
Prediction of alloying windows and alloying routes with a 3D structure map
Big-Data driven Materials Science Workshop, Lausanne, Switzerland

14.09.2017
J. Rogal
Atomistic mechanisms and kinetics during phase transformations in metals
Psi-k Workshop on Theory and Simulation Challenges of Nano Phase-Change Materials, Coventry, UK

19.09.2017
H. u. Hassan, W. Ye, A. Hartmaier
Micromechanical modeling of fatigue crack initiation in aluminium 2024
EUROMAT 2017, Thessaloniki, Greece

20.09.2017
I. Steinbach
Atomistically informed full-field simulation of tempered martensite: Quenching, tempering and mechanical characterization
EUROMAT 2017, Thessaloniki, Greece

20.09.2017
R. Drautz
From density functional theory to analytic magnetic bond-order potentials and the calculation of thermodynamic properties
EUROMAT 2017, Thessaloniki, Greece

22.09.2017
J. Neugebauer, T. Hickel
Modelling structural materials in realistic environments by ab initio thermodynamics
EUROMAT 2017, Thessaloniki, Greece

08.10.2017
B. Grabowski, C. Race, J. Neugebauer
Atomistic simulations on grain boundary migration
MS&T, Pittsburgh, USA

09.10.2017
J. Neugebauer, T. Hickel, Z. Pei, J. Janßen
Materials discovery and design at finite temperatures
MS&T, Pittsburgh, USA

11.10.2017
S. Münstermann, B. Döbereiner, D. Novokshanov
Design of damage tolerance in high-strength steels
MPA-Seminar, Stuttgart, Germany

16.10.2017
M. Todorova, A. K. Vatti, S. Yoo, J. Neugebauer
Free energy sampling for electrochemical systems
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, University of California, Los Angeles, USA

16.10.2017
J. Neugebauer
Free energy sampling strategies for structurally complex materials
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, University of California, Los Angeles, USA

16.10.2017
J. Neugebauer
Stochastic sampling and accelerated time dynamics on multidimensional surfaces
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, University of California, Los Angeles, USA

17.10.2017
J. Rogal
Finding reaction coordinates for phase transformations in metals
Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, University of California, Los Angeles, USA

06.11.2017
M. Mrovec
Atomistic simulations of extended defects using coarse-grained electronic structure methods
Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

14.11.2017
I. Stockem
The interaction of spin dynamics and lattice vibrations of CrN in the paramagnetic state
BIfAM Seminar, Bielefeld, Germany

21.11.2017
B. Dutta, F. Körmann, J. Neugebauer, T. Hickel
Temperature-driven effects in functional materials: Ab initio insights
Université Pierre and Marie Curie, Paris, France

28.11.2017
J. Rogal
Finding reaction coordinates during phase transformations in solids
MRS Fall Meeting, Boston, USA

04.12.2017
B. Grabowski
Knowledge driven engineering of metals: Development and application of ab initio based scale bridging methods
TU Delft, Netherlands

10.01.2018
A. Glensk
From thermodynamics to phonon lifetimes: Anharmonic calculations with ab initio accuracy
CECAM workshop: Anharmonicity and thermal properties of solids, Paris, France

31.01.2018
R. Drautz
From the atomic interaction to thermodynamic and mechanical properties of materials
Physikalisches Kolloquium, TU Chemnitz, Germany

02.02.2018
J. Rogal
Atomistic insight into the dynamics and mechanisms of phase transformations in metals
Penn Institute for Computational Science Colloquium, Philadelphia, USA

08.02.2018
I. Steinbach
Why Phase-Field?
5th GAMM Workshop on Phase-field Modelling, TU Dresden, Germany

09.02.2018
J. Rogal
Atomistic insight into the dynamics and mechanisms of phase transformations in materials
NYU Chemistry Seminar, New York University, USA

15.02.2018
B. Dutta, F. Körmann, T. Hickel, J. Neugebauer
Role of temperature dependent excitations and the coupling between them in functional materials: Ab initio insights
Linköping University, Sweden

15.02.2018
P. Dey, T. Hickel, J. Neugebauer
Understanding hydrogen embrittlement based on ab initio methods
Linköping University, Sweden

23.02.2018
S. G. Fries
Magnetic degrees of freedom, state of the art first-principles/CALPHAD modeling approaches
IMR Seminar, Tohoku University, Sendai, Japan

26.02.2018
T. Hickel, I. Bleskov, P. Dey, F. Körmann, B. Grabowski, J. Neugebauer
Strengthening mechanisms in a precipitation hardened high-Mn lightweight steel
6th ESISM Workshop on Fundamental Issues of Structural Materials, Kyoto, Japan

26.02.2018
J. Neugebauer, M. Todorova, B. Grabowski, T. Hickel, G. P. Leyson
Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach
Max-Planck-Institut für Plasmaphysik, Garching, Germany

26.02.2018
B. Grabowski, S. Hadian, A. Nematollahi, C. Kirchlechner, G. Dehm, J. Neugebauer, W. Ko, J. B. Jeon
Dislocation twin boundary interactions in nanoscale Cu bi-crystals: Simulation versus experiment
Schöntal Symposium – Dislocation based Plasticity, Schöntal, Germany

07.03.2018
I. Steinbach
Multi-scale simulation of Ni-base turbine blades: From solidification to rafting under creep conditions
Industrial Colloquium of the SFB/TR103, Fürth, Germany

11.03.2018
J. Neugebauer, J. Janßen, F. Körmann, B. Grabowski, T. Hickel
Exploration of large ab initio data spaces to design structural materials with superior mechanical properties
Hume-Rothery Award Symposium, TMS Conference, Phoenix, USA

11.03.2018
T. Hickel, J. Neugebauer, F. Körmann, B. Grabowski, M. Todorova
Modelling structural materials in realistic environments by ab initio thermodynamics
TMS conference, Phoenix, USA

12.03.2018
B. Grabowski, J. Neugebauer
Efficient and accurate computation of melting temperatures and enthalpies and entropies of fusion from ab initio
TMS conference, Phoenix, USA

26.03.2018
S. G. Fries
Magnetic degrees of freedom, state of the art first-principles/CALPHAD modeling approaches
Laboratory of Semiconductor Materials, EPFL, Lausanne, Switzerland

29.03.2018
I. Steinbach
Why Phase-field?
Hong Kong University of Science and Technology, Hong Kong, China

29.03.2018
J. Rogal
Interstitial and substitutional diffusion in metals
International Seminar series on Time Dependent Multiscale Phenomena of Materials Tohoku University, Sendai, Japan

29.03.2018
M. Grabowski, J. Rogal, R. Drautz
Modelling diffusion in non-dilute Ni-Re alloys: A combined kinetic Monte Carlo and cluster expansion approach
International Seminar series on Time Dependent Multiscale Phenomena of Materials, Tohoku University, Sendai, Japan

29.03.2018
M. Mrovec
Atomistic simulations of extended defects using coarse-grained electronic structure methods
Masaryk University, Brno, Czech Republic

03.04.2018
J. Neugebauer, L. Zhu, F. Körmann, B. Grabowski, T. Hickel
From electrons to the design of structurally complex materials
SFB ViCoM conference EPT 2018: From electrons to phase transitions, Vienna, Austria

10.04.2018
M. Todorova, S. Surendralal, S. Yoo, J. Neugebauer
Atomistic insights into surface stability and reactivity at solid/liquid interfaces from first principles calculations
Technical University Vienna, Austria

16.04.2018
T. Hickel, A. Glensk, R. Nazarov, U. Aydin, B. Grabowski, O. Hedge, J. Neugebauer
Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction
2018 Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments, Trieste, Italy

23.04.2018
R. Drautz
From the atomic interaction to thermodynamic and mechanical properties of materials
45th International Conference on Metallurgical Coatings and Thin Films, San Diego, USA

24.04.2018
I. Roslyakova, S. Zomorodpoosh, A. Obaied, Y. Jiang, L. Zhang, R. Otis, B. Bocklund
Third generation CALPHAD databases by automated statistical regression analysis
HERO-M Seminar, KTH Royal Institute of Technology, Stockholm, Sweden

25.04.2018
I. Roslyakova, I. Steinbach
Property models for Ni-based superalloys: Physically-based and statistical modelling approaches
Thermo Calc Software AB, Solna, Sweden

18.05.2018
B. Grabowski
Knowledge driven engineering of materials: Development and application of ab initio based scale bridging methods
Helmut-Schmidt-Universität Hamburg, Germany

01.06.2018
T. Hickel
Characterizing complex materials by ab initio methods
Abteilungskolloquium, BAM Berlin, Germany

14.06.2018
R. Drautz
From electrons to interatomic interactions and to properties of materials
Kolloquium SFB 716, Universität Stuttgart, Germany

14.06.2018
T. Hickel, B. Grabowski, F. Körmann, A. Glensk
Understanding phase stabilities and microstructure formation with finite temperature ab initio methods
MPIE Lecture Series, Düsseldorf, Germany

04.07.2018
T. Hammerschmidt, M. Čák, J. Jenke, A. C. Ladines, Y. Lysogorskiy, A. P. Subramanyam, N. Wang, R. Drautz
Parameterisation and transferability of analytic bond-order potentials
Modern Approaches to Coupling Scales In Materials Simulations Workshop, Lenggries, Germany

04. 07. 2018
S. G. Fries
High temperature, high expectations
XVI International IUPAC conference on high temperature materials chemistry (HTMC-XVI), Ekaterinburg, Russia

08. 07. 2018
O. Waseda
Machine-learning assisted Heisenberg model for systems with ill-defined magnetic interactions
Thermec 2018 Conference, Paris, France

10. 07. 2018
T. Hickel, P. Dey, B. Dutta, M. Friák, J. Neugebauer
Phase stability and chemical composition of nano precipitates: A first principles study for the example of κ carbides
Thermec 2018 Conference, Paris, France

11. 07. 2018
J. Neugebauer, S. Hadian, L. Huber, C. Race, B. Grabowski
Modelling thermodynamics and kinetics of general grain boundaries: Challenges and successes
Thermec 2018 Conference, Paris, France

11. 07. 2018
R. Drautz
Analytic bond-order potentials for transition metals
David Pettifor Scientific Symposium, Oxford, UK

11. 07. 2018
M. Mrovec
Atomistic simulations of extended defects using bond-order potentials
David Pettifor Scientific Symposium, Oxford, UK

11. 07. 2018
T. Hammerschmidt, B. Seiser, A. Bialon, J. Koßmann, J. Jenke, A. P. Subramanyam, Y. Lysogorskiy, D. G. Pettifor, R. Drautz
Prediction of structural stability with structure maps
David Pettifor Scientific Symposium, Oxford, UK

12. 07. 2018
I. Steinbach
Phase-field and CALPHAD
2018 SIAM Conference on Mathematical Aspects of Material Science, Portland, USA

12. 07. 2018
I. Roslyakova, I. Steinbach
Third generation CALPHAD databases by automated statistical regression analysis
2018 SIAM Conference on Mathematical Aspects of Material Science, Portland, USA

19. 07. 2018
J. Rogal
Extended timescale simulations of atomistic processes during phase transformations in materials
CRC 1114 – Colloquium, FU Berlin, Germany

03. 09. 2018
T. Hammerschmidt, B. Seiser, A. Bialon, J. Koßmann, D. G. Pettifor, R. Drautz
Navigating chemical compound space with structure maps
Materials Discovery Symposium, Liverpool, UK

09. 09. 2018
M. Mrovec
Atomistic studies of dislocations in iron using magnetic bond-order potential
Multiscale Modelling of Materials for Sustainable Development Conference, Vietnam National University, Hanoi, Vietnam

13. 09. 2018
A. Hartmaier
What does nanoindentation teach us on macroscopic material behavior
Indentation 2018, Liège, Belgium,

26. 09. 2018
Y. Lysogorskiy
Locally approximated electronic structure based descriptors for predicting materials properties
A hands-on course on tools for novel-materials discovery, Lausanne, Switzerland

01. 10. 2018
J. Rogal
Analysis of reaction coordinates for nucleation in metals
E-CAM State-of-the Art Workshop: Large Scale Activated Event Simulations, Vienna, Austria

10.10.2018
T. Hammerschmidt
Analytic bond-order potentials: From downfolding DFT eigenspectra to large-scale atomistic simulations
Frontiers in Molecular Dynamics: Machine Learning, Deep Learning and Coarse Graining Workshop, Tel-Aviv, Israel

12.10.2018
I. Steinbach, M. A. Ali, J. V. Görler
Full-field simulation of Ni-base turbine blades: From precipitation to rafting and under creep conditions
Society of Engineering Sciences 2018, Madrid, Spain

15.10.2018
J. Neugebauer, L. Zhu, F. Körmann, B. Grabowski, T. Hickel
Data driven approaches in materials design: Theory meets experiment
RCTP-2018 Conference, Moscow, Russia

18.10.2018
S. G. Fries, U. R. Kattner
Effective bond energy formalism in the multi-component CALPHAD approach: An improvement of TCP phases descriptions based on first-principles data
Hero-m 2i, KTH, Stockholm, Sweden

26.10.2018
J. V. Görler, M. A. Ali, O. Shchyglo, I. Steinbach
Simulation of rafting and topological inversion in Ni-base superalloys
2018 KIM Fall Conference: Symposium on Microstructure Modeling of Materials, Daejeon, South Korea

26.10.2018
I. Steinbach, M. A. Ali, O. Shchyglo, C. Koerner
Stress-strain evolution during rapid solidification and self-tempering of additive manufactured Ni-base superalloys simulated by a mesoscopic phase-field model
2018 KIM Fall Conference: Symposium on Microstructure Modeling of Materials, Daejeon, South Korea

28.10.2018
J. Neugebauer, J. Janßen, F. Körmann, B. Grabowski, T. Hickel
Exploration of large ab initio data spaces to design structural materials with superior mechanical properties
9th International Conference on Multiscale Materials Modeling, Osaka, Japan

30.10.2018
M. Todorova, S. Yoo, S. Surendralal, J. Neugebauer
Ab initio modelling of solid/liquid interfaces: Challenges and insights
FS Seminar, DESY, Hamburg, Germany

31.10.2018
J. Rogal
Atomistic processes at interfaces on extended timescales
9th International Conference on Multiscale Materials Modeling, Osaka, Japan

31.10.2018
I. Steinbach
Atomistically informed full-field simulation of tempered martensite: Quenching, tempering and mechanical characterization
9th International Conference on Multiscale Materials Modeling, Osaka, Japan

08.11.2018
J. Neugebauer
Electronic structure and computational metallurgy
EMMC expert meeting and roadmap, CECAM-HQ-EPFL, Lausanne, Switzerland

21.11.2018
R. Drautz
From electrons to properties of materials
8th NRW Nano Conference, Dortmund, Germany

ICAMS

Collaborations, Guests and Vistiors

17. Collaborations, Guests and Visitors

Dr. Alessio Alexiadis
School of Chemical Engineering
University of Birmingham
Birmingham, UK
27.02.2018

Prof. Dr. Alan Ardell
Department of Materials Science and Engineering
University of California, Los Angeles
Los Angeles, USA
26.03.2017-31.03.2017

Prof. Dr. Mark Asta
Department of Materials Science and Engineering
University of California, Berkeley
Berkeley, USA
25.06.2018-27.06.2018

Prof. Dr. Irene J. Beyerlein
Mechanical Engineering Department,
Materials Department
University of California, Santa Barbara
Santa Barbara, USA
25.06.2018-27.06.2018

Prof. Dr. Erik Bitzek
Department of Materials Science and Engineering
Friedrich-Alexander Universität Erlangen-Nürnberg
Erlangen, Germany
28.03.2017-31.03.2017, 27.04.2018-30.04.2018

Brandon Bocklund
Department of Materials Science and Engineering
Pennsylvania State University
University Park, USA
06.11.2017-17.11.2017

Dr. Mark Jon Cawkwell
Theoretical Division Group T-1
Los Alamos National Laboratory
Los Alamos, USA
12.07.2018-04.08.2018

Prof. Dr. Long-Qing Chen
Department of Materials Science and Engineering
Pennsylvania State University
University Park, USA
25.06.2018-27.06.2018

Prof. Dr. Ying Chen
Department of Finemechanics, and Fracture and
Reliability Research Institute
Tohoku University
Sendai, Japan
11.10.2017-14.10.2017

Dr. Jean-Philippe Couzinié
Institut de Chimie et des Matériaux
Université Paris-Est
Thiais, France
11.01.2018

Prof. Dr. Stefano Curtarolo
Department of Mechanical Engineering and Materials Science
Duke University
Durham, USA
19.02.2018

Prof. Dr. William Curtin
Laboratoire de modélisation mécanique multi-échelle
École Polytechnique Fédérale de Lausanne
Lausanne, Switzerland
25.06.2018-27.06.2018

Dr.-Ing. Reza Darvishi Kamachali
Microstructure physics and alloy design
Max-Planck-Institut für Eisenforschung
Düsseldorf, Germany
25.06.2018-27.06.2018

M.Sc. Theresa Anne Davey
Department of Finemechanics, and Fracture and Reliability Research Institute
Tohoku University
Sendai, Japan
27.01.2017-03.02.2017

Prof. Dr. René de Borst
Department of Civil and Structural Engineering
University of Sheffield
Sheffield, UK
29.06.2018

Dr. Peter Derlet
Condensed Matter Theory Group
Paul Scherrer Institute
Villigen, Switzerland
22.06.2017

Prof. Dr. Antonín Dlouhý
Institute of Physics of Materials
Academy of Sciences of the Czech Republic
Brno, Czech Republic
25.06.2018-27.06.2018

Prof. Dr. Yong Du
State Key Laboratory of Powder Metallurgy
Central South University (CSU)
Changsha, China
25.06.2018-27.06.2018

Prof. Dr. Christian Elsässer
Materialmodellierung
Fraunhofer-Institut für Werkstoffmechanik IWM
Freiburg, Germany
10.01.2018-11.01.2018

Dr.-Ing. Philipp Simon Engels
Siemens AG
Mülheim/Ruhr, Germany
30.05.2018

Dr.-Ing. Alexander Epishin
Institut für Werkstoffwissenschaften und -technologien
TU Berlin, Berlin
Germany
02.02.2017

Dr.-Ing. Bernard Fedelich
Experimentelle und modellbasierte Werkstoffmechanik
Bundesanstalt für Materialforschung und -prüfung
Berlin, Germany
29.03.2017-31.03.2017

Prof. Dr. Michael Finnis
Department of Materials
Imperial College London
London, UK
01.08.2017-31.08.2017, 05.09.2017-16.09.2017, 01.06.2018-30.06.2018

Patrick Fopp
Institut für Materialphysik im Weltraum
DLR
Köln, Germany
25.06.2018-27.06.2018

Dr. Martin Friák
Department of Structure of Materials
Academy of Sciences of the Czech Republic
Brno, Czech Republic
15.02.2017-17.02.2017

Prof. Dr. Easo George
Department of Materials Science and Engineering
University of Tennessee
Knoxville, USA
20.12.2018

Dr. Anna Grünebohm
Theoretische Physik
University Duisburg-Essen
Duisburg, Germany
13.07.2017, 25.06.2018-27.06.2018

Prof. Dr. Anne Marie Habraken
Department of Architecture, Geology,
Environment & Constructions
Université de Liège
Liège, Belgium
22.11.2018

Dr.-Ing. Stefanie Hanke
Werkstofftechnik
Universität Duisburg-Essen
Duisburg, Germany
06.12.2018

Prof. Dr. Andreas Heuer
Institut für Physikalische Chemie
Universität Münster
Münster, Germany
05.07.2018

Dr. Hendrik Hölscher
Institute of Microstructure Technology
Karlsruhe Institute of Technology (KIT)
Eggenstein-Leopoldshafen, Germany
29.06.2017

Prof. Dr. Norbert Huber
Materials Mechanics Division
Helmholtz-Zentrum Geesthacht
Geesthacht, Germany
12.04.2018

Prof. Dr. Haruyuki Inui
Department of Materials Science and Engineering
Kyoto University
Kyoto, Japan
28.03.2017-01.04.2017

Dr. Eric Jägle
Alloys for Additive Manufacturing group
Max-Planck Institut für Eisenforschung
Düsseldorf, Germany
27.04.2017

Prof. Dr. Florian Kargl
Institut für Materialphysik im Weltraum
DLR
Köln, Germany
25.06.2018-27.06.2018

Dr. James Kermode
School of Engineering
University of Warwick
Coventry, UK
28.03.2017-31.03.2017

Manuel Köbrich
Allgemeine Werkstoffeigenschaften
Friedrich-Alexander Universität Erlangen-Nürnberg
Erlangen
Germany
07.08.2018-10.08.2018

Prof. Dr. Dennis Kochmann
Department of Mechanical and Process Engineering
ETH Zürich
Zürich, Switzerland
25.06.2018-27.06.2018

Prof. Dr.-Ing. Carolin Koerner
Department of Materials Science and Engineering
Friedrich-Alexander Universität Erlangen-Nürnberg
Erlangen, Germany
26.01.2017, 29.03.2017-31.03.2017

Dr. Ute Kolb
Institut für Physikalische Chemie
Johannes Gutenberg-Universität Mainz
Mainz, Germany
12.01.2017

Dr. Yi Kong
State Key Laboratory of Powder Metallurgy
Central South University (CSU)
Changsha, China
25.06.2018-19.08.2018

Dr. Jörg Koßmann
Clouth Sprenger GmbH
Moers, Germany
30.05.2018

Rakesh Kumar
Department of Physics
Indian Institute of Technology Ropar
Ropar, India
29.10.2018-14.11.2018

Prof. Dr. Khanh Chau Le
Lehrstuhl für Allgemeine Mechanik
Ruhr-Universität Bochum
Bochum, Germany
02.08.2017

Dr. Christian Leinebach
Advanced Materials Processing
Empa
Dübendorf, Switzerland
07.09.2017

Dr. Erica Lilleodden
Experimental Materials Mechanics
Helmholtz-Zentrum Geesthacht
Geesthacht, Germany
06.07.2017

Dr. Yi-Shen Lin
Department of Materials Science and Engineering
University of Pennsylvania
Philadelphia, USA
01.02.2017-15.02.2017

Prof. Javier Llorca
IMDEA Materials Institute
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Getafe, Madrid, Spain
25.06.2018-27.06.2018

Prof. Dr. Yong Lu
Shengnuo Research Institute of Non-ferrous Metal Materials
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Xiamen, China
21.06.2017-30.06.2017

Runsen Ma
Department of Materials
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Oxford, UK
03.07.2017-26.07.2017

Prof. Dr.-Ing. Lutz Mädler
IWT Verfahrenstechnik
Universität Bremen
Bremen, Germany
14.06.2018

Dr. Phillip Michael Maffettone
Department of Chemistry
University of Liverpool
Liverpool, UK
29.10.2018-14.11.2018

Mustafa Mamduh Mustafa Awd
Fakultät Maschinenbau Werkstoffprüftechnik
TU Dortmund
Dortmund, Germany
25.06.2018-27.06.2018

Dr.-Ing. Hong Mao
Faculty of Mechanical Engineering
Central South University (CSU)
Changsha, China
01.07.2017-30.08.2017

Dr. Anika Marusczyk
Business Department
Robert Bosch GmbH
Renningen, Germany
22.06.2018

Dr. Dmitry Medvedev
Departement of Scalebridging Thermodynamic and Kinetic Simulation
Lavrentyev Institute of Hydrodynamics
Novosibirsk, Russian Federation
06.01.2017-06.02.2017, 08.01.2018-02.02.2018

Jan Inge Meling
Department of Mechanical and Industrial Engineering
NTNU Norwegian University of Science and Technology
Bochum, Germany
11.06.2018-15.06.2018

Dr. Edern Menou
Institut des matériaux Jean Rouxel
Safran Tech
Magny-les-Hameaux, France
25.06.2018-27.06.2018

Prof. Dr. Matthias Militzer
Department of Materials Engineering
The University of British Columbia
Vancouver, Canada
17.12.2018

Prof. Dr. Tetsuo Mohri
Center for Computational Materials Science
Tohoku University
Sendai, Japan
24.01.2017-26.01.2017

Alexander Müller
Materials Science and Engineering for Metals
Friedrich-Alexander Universität Erlangen-Nürnberg
Erlangen, Germany
25.06.2018-27.06.2018

Prof. Dr. Eckehard Müller
Fachbereich Mechatronik und Maschinenbau
Hochschule Bochum
Bochum, Germany
25.06.2018-27.06.2018

Prof. Dr. Lucia Nicola
Department of Materials Science and Engineering
Delft University of Technology
Delft, Netherlands
30.11.2017

Kapil Chandra Nidadavolu
Indian Institute of Technology Madras
Chennai, India
16.05.2018-25.07.2018

Prof. Dr.-Ing. Thomas Niendorf
Institut für Werkstofftechnik
Universität Kassel
Kassel, Germany
21.06.2018

Prof. Dr. Gregory B. Olson
Materials Science and Engineering
Northwestern University, QuesTek Innovations LLC
Evanston, USA
25.06.2018-28.06.2018

Dr. Richard Otis
Engineering and Science Directorate
California Institute of Technology
Pasadena, USA
29.05.2017-09.06.2017

Dr. Salvador Pané i Vidal
Multi-Scale Robotics Lab
ETH Zurich
Zurich, Switzerland
23.01.2017

Dr. Jiwon Park
Korea Institute of Materials Science (KIMS)
Changwon, Republic of Korea
04.09.2017-31.10.2017

Prof. Dr. Anthony T. Paxton
Department of Physics
King's College London
London, UK
07.03.2018-10.03.2018

Dr. Yingbiao Peng
State Key Laboratory of Powder Metallurgy
Central South University (CSU)
Changsha, China
25.06.2018-19.08.2018

Prof. Dr.-Ing. Bernhard Peters
Department of Engineering
University of Luxembourg
Esch-sur-Alzette, Luxembourg
14.11.2017

Dr. Evgeny Pogorelov
Faculty of Production Engineering
Universität Bremen
Bremen, Germany
09.01.2018

Dr. Florian Pyczak
Institute of Materials Research
Helmholtz-Zentrum Geesthacht
Geesthacht, Germany
07.12.2017

Prof. Dr. Eugen Rabkin
Department of Materials Science and Engineering
Technion - Israel Institute of Technology
Haifa, Israel
25.06.2018-27.06.2018

Prof. Dr. Catherine Rae
Department of Materials Science and Metallurgy
University of Cambridge
Cambridge, UK
29.03.2017-31.03.2017

Dr.-Ing. Ali Ramazani
Mechanical Engineering
Massachusets Institute of Technology
Cambridge, USA
29.10.2018-11.11.2018

Dr. Kyle Ramos
High Explosives Science and Technology
Los Alamos National Laboratory
Los Alamos, USA
16.07.2018-19.07.2018

Dennis Rapp
Institute for Materials Testing, Materials Science and Strength of Materials (IMWF)
Universität Stuttgart
Stuttgart, Germany
25.06.2018-27.06.2018

Dr. Jens Reiser
Applied Materials Physics
Karlsruhe Institute of Technology (KIT)
Eggenstein-Leopoldshafen, Germany
04.12.2017-08.12.2017

Prof. Dr. Markus Rettenmayr
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