Scientific Report 2019 and 2020

ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS

Scientific Report 2019 and 2020

ICAMS
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Preface

This report gives an overview of our research and teaching activities in the past two years and the current structure of ICAMS.

Our institute has grown. Two new junior professors have been appointed, Professor Anna Grünebohm for "Scale-bridging Simulation of Functional Composites" and Professor Markus Stricker "Materials Informatics and Data Science". Their research will complement and extend our research portfolio and we look forward to working with them. Furthermore, a new Advanced Study Group from the Faculty of Civil Engineering at Ruhr-Universität Bochum strengthens our expertise in "Computational Mechanics".

We look back on two years of intense research collaborations with our university-wide, regional, national and international partners and stimulating scientific exchange in seminars, workshops and conferences.

In 2020 both staff members and students were heavily influenced in their everyday work and studies by the Covid-19 pandemic. We wish to thank everyone at ICAMS, Ruhr-Universität Bochum and our partner institutions who contributed with their patience, dedication and ideas, not only to make the best of the situation, but growing from it by giving impulses for new ways of digital teaching and collaboration.

We are grateful to our research partners from academia and industry worldwide, the funding agencies, in particular Deutsche Forschungsgemeinschaft, for making our work possible and thank the members of our scientific advisory board for their support. Finally, our gratitude goes to all the present and past members of ICAMS for successfully advancing materials modelling and simulation.

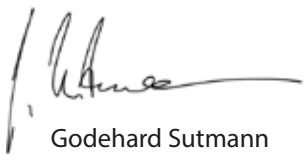
Ingo Steinbach
Managing Director

Ralf Drautz

Anna Grünebohm

Alexander Hartmaier

Markus Stricker



Godehard Sutmann

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ICAMS in 2019 and 2020

2. ICAMS in 2019 and 2020

▸ ICAMS in 2019 and 2020

The appointment of two new professors, Prof. Dr. Anna Grünebohm and Prof. Dr. Markus Stricker marks two milestones for advancing scale-bridging materials simulation at ICAMS. New research projects have been started, several of which are described in the corresponding departments' chapters. A new Advanced Study Group, "Computational Mechanics," headed by Prof. Dr. Daniel Balzani and Prof. Dr. Klaus Hackl from the Faculty of Civil Engineering at RUB, has been established to strengthen the growing number of research collaborations and joint teaching activities in this field. We have been receiving a steeply rising number of applications to our masters course "Materials Science and Simulation", making it one of the most successful international study programmes at RUB. The graduate school for "Scalebridging Materials Simulation" was launched at ICAMS in fall 2020 to foster young scientists' interdisciplinary research. Also, ICAMS will take a leading part in a new bachelor's program "Materialwissenschaft" (Materials Science), starting in 2021.

The following sections provide a summary of the ICAMS activities.

▸ New Professors and Lecturers

Anna Grünebohm, who came to ICAMS in May 2019 as leader of the Emmy Noether Group "Scale-bridging computational design of multifunctional ferroelectric composites" was appointed junior professor by the faculty of mechanical engineering. Since then, she has been head of the independent research group with the same name, thus complementing ICAMS' research portfolio with her expertise in this important class of functional materials.

Markus Stricker joined ICAMS in July 2020 as a junior professor for "Materials Informatics and Data Science." Both areas are internationally rapidly evolving fields that open new research perspectives at ICAMS and will strengthen ICAMS teaching in the area.

Jutta Rogal and Thomas Hammerschmidt completed their habilitations at the faculty of physics in summer 2020.

Fig. 2.1: Prof. Dr. Anna Grünebohm and Prof. Dr.Markus Stricker lead the two new groups at ICAMS (Photos Katja Maquard, RUB).

▸ Workshops and Conferences

ICAMS organised and contributed to the organisation of several workshops and conferences in the past two years.

In April 2019, "Hydrogen in Metals – Current Understanding and Future Needs" took place at Oxford University. The "Phasefield 19" conference was jointly organised by ICAMS' STKS department and Yunzhi Wang from Ohio State University in May 2019 and attracted more than 170 participants from 20 countries. In the same month, the ICAMS Advanced Discussions were dedicated to Data-oriented Materials Science and brought together materials scientists from academia and industry. The international symposium "Superalloy Data Science 2020" took place in January 2020 at Ruhr-Universität Bochum and focused on data acquisition, storage and mining, and machine learning.

Furthermore, ICAMS scientists were members of the scientific panels or contributed to the organisation of conferences and workshops, including symposia at E-CAM 2019, HEMS, EUROMAT 2019, MSE 2020 and TOFA 2020.

Fig. 2.2: The PF19 conference took place in April 2019 at RUB.

Fig. 2.3: Participants of the Superalloy Data Science Symposium 2020.

▸ Teaching

Bachelor program in Materials Science

A new Bachelor course "Materialwissenschaft" will be launched in the winter term 2021/22. The curriculum has been jointly developed by ICAMS and the Institute for Materials, and the faculty of Mechanical Engineering will host the course. Students will acquire a solid background in scientific, engineering, mathematical and programming knowledge. The course programme is unique in our region, and thus ICAMS is among the first German universities to meet the growing demand for expertise in this field. Students can either specialise in "Modelling and Simulation" or "Experimental Materials Science" during the programme, which will qualify them for a career as materials scientists in industry or for advanced studies in our master's programme "Materials Science and Simulation", the master's programme "Mechanical Engineering" at RUB, or similar courses at other academic institutions. Further information can be found at www.mawi.rub.de.

Fig. 2.4: Visit the website of our new Bachelor course at www.mawi.rub.de.

Master's course Materials Science and Simulation (MSS)

In 2019 we received more than 1400, and in 2020, almost 1500 applications for our master's programme "Materials Science and Simulation." Altogether 57 students eventually took up their studies in the last two years. 10 master's students successfully graduated in 2019 and 22 in 2020.

ICAMS regularly organises excursions to bring MSS students into contact with companies in Germany. The 2019 tour led us to Hamburg and Bremen, including visits to DLR, Volkswagen AG, Helmholtz Zentrum Geesthacht and IWT Bremen.

Fig. 2.5: ICAMS Students on tour during their 2019 excursion.

Regular "fireplace talks," at which 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. The 2019 and 2020 fireplace talks hosted Behshid Azimi Manavi from Robert Bosch GmbH, Stuttgart and Anna-Lena Kauws from TRIMET Aluminium SE, Essen.

Fig. 2.6: A typical teaching situation in 2020.

Fig. 2.7: Production of a video for the first semester students

▸ Online Teaching

The outbreak of the COVID pandemic has brought significant changes and challenges to our teaching. Suitable online tools and formats have been identified for lectures, exams and other curricular activities to offer our students a reasonable alternative to face-to-face classroom teaching. RUB's centre for teaching and learning (ZfW), the RUB E-learning team and RUB IT. Services provided methodological and technical support, including video conference software and extended E-learning platforms. ICAMS equipped its seminar room with up-to-date video and audio streaming equipment to allow live remote teaching and courses recording. With the beginning of the winter term 2020/2021, the situation has got more complex; as most of the admitted first-semester students could not obtain a visa due to the pandemic, our online teaching methods covered time zones from Taiwan to Brazil.

In a university-wide competition, ICAMS won funding for a project to support our master's course freshmen. We developed the digital format "4 for U," in which tutors from higher semesters assist the first-semester students in technical and organisational questions.

▸ Graduate School

In 2020 ICAMS has established a Graduate School on scale-bridging materials modelling, targeting doctoral candidates with a research focus on materials modelling. The programme's core is a lecture series offered by the three ICAMS departments, introducing graduate students to the crucial simulation methods for the corresponding length scales. Another focus is scientific exchange and soft skills development, including team building, scientific writing, and communicating science, which is realised through joint PhD seminars and presentations on external conferences and workshops. The programme is complemented by non-subject-specific and cross-disciplinary courses offered by RUB Research School.

Fig. 2.8: Suzana G. Fries obtained the Hume Rothery Prize of IOM³ in 2019.

Fig. 2.9: Anna Grünebohm obtained the 2020 Innovation Award of the state North Rhine-Westphalia, © MWIDE NRW/Susanne Kurz.

▸ Awards

Anna Grünebohm was awarded the Innovation Prize of the State of North Rhine-Westphalia in the young talent category. The prize is endowed with € 50,000. Suzana G. Fries obtained the Hume Rothery Prize of IOM³ in 2019. Rebecca Janisch received an "Outstanding Reviewer" award for excellence in reviewing in 2018, as selected by the Editors of Acta Materialia and Scripta Materialia. Yanyan Liang won a poster award at the Mainz Materials Simulation Days 2019.

▸ Publications

In 2019 and 2020, ICAMS researchers, including researchers of the ICAMS Advanced Study Groups, published more than 200 papers. Furthermore, 16 theses were completed by our PhD students, and 29 Master theses were supervised or co-supervised in 2019 and 2020. *Figure 2.10* shows the number of publications since 2008. A detailed list of all publications from the last two years can be found in chapter 14.

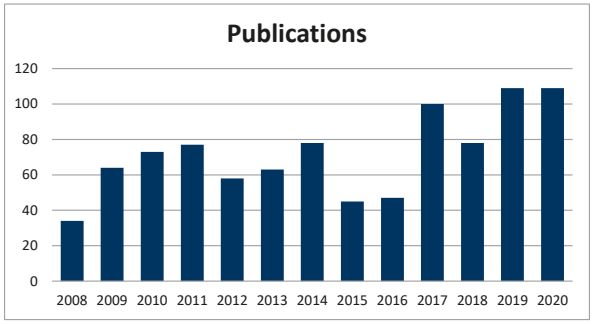

Fig. 2.10: ICAMS publications since 2008.

ICAMS

Organisation of ICAMS

3. Organisation of ICAMS

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Chair: Prof. Dr. Ingo Steinbach

Micromechanical and Macroscopic Modelling
Chair: Prof. Dr. Alexander Hartmaier

▶ ICAMS Independent Research Groups

Scale-bridging Simulation of Functional Composites
Prof. Dr. Anna Grünebohm

Materials Informatics and Data Sciece
Prof. Dr. Markus Anthony Stricker

High Performance Computing in Materials Science
Prof. Dr. Godehard Sutmann

▶ Advanced Study Groups

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Input Data and Validation
Lehrstuhl Werkstoffwissenschaft, RUB
Chair: Prof. Dr.-Ing. Gunther Eggeler

Processing and Characterization
Institut für Eisenhüttenkunde, RWTH Aachen
Chair: Prof. Dr.-Ing. Ulrich Krupp

Diffusion and Microstructure Analysis
Institut für Materialphysik, WWU Münster
Chair: Prof. Dr. Gerhard Wilde

Continuum Mechanics
Lehrstühle Kontinuumsmechanik/Materialtheorie, RUB
Chairs: Prof. Dr.-Ing. Daniel Balzani, Prof. Dr. Klaus Hackl

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ICAMS

Department Atomistic Modelling and Simulation AMS

4. Department Atomistic Modelling and Simulation

Prof. Dr. Ralf Drautz

▸ Research

Within the materials 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. We obtain effective interatomic potentials by combining electronic structure theory and mathematical analysis with large data sets.

2. We employ interatomic potentials in atomistic simulations for insight into and understanding of materials properties.

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

Atomistic simulations focus on predicting structural and mechanical properties of materials, on rare event dynamics and on computing phase diagrams. 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 re-parameterize 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)
- Data-driven methods for atomistic simulations (Dr. Yury Lysogorskiy)
- Atomistic simulation of the kinetics of phase transformations (Dr. Jutta Rogal, until September 2020)

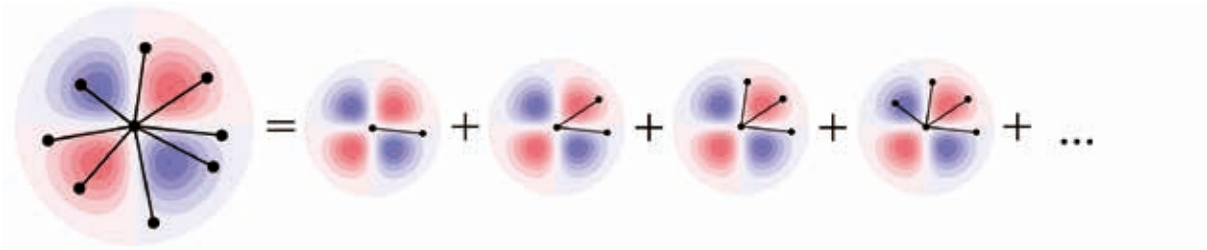


Fig. 4.1: Illustration of the atomic cluster expansion.

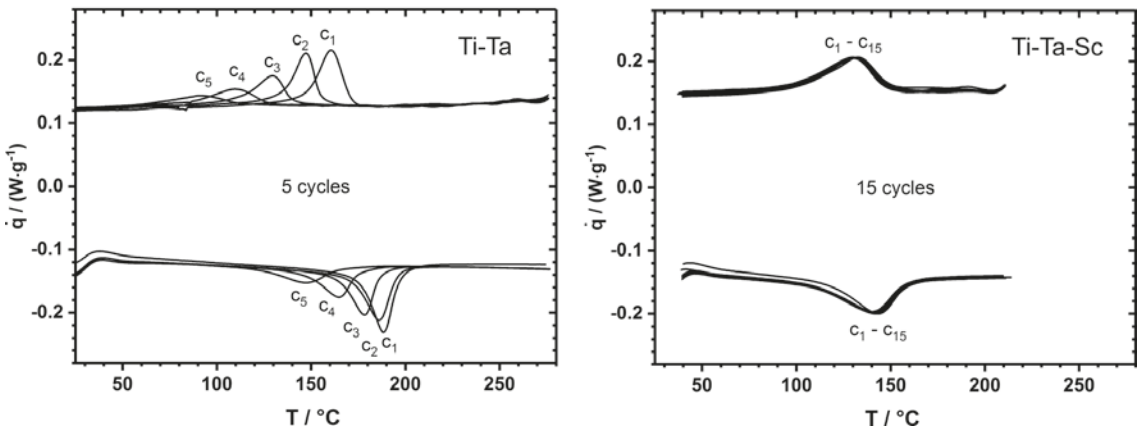


Fig. 4.2: Computational design of a novel high-temperature shape memory alloy. Fast degradation of the original alloy (left) vs. stable cycling of the predicted alloy (right).

AMS

4.1. Atomistic Simulation of Structural and Phase Stability

Group leader:
Dr. Thomas Hammerschmidt

Group members:
Aleksei Egorov
Dr. Mariano Forti
Isabel Pietka
Senja Josepha Johanna Ramakers

▸ 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 and superalloys). 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 and machine-learning as complementary data-driven methods. The TB and BOP models are obtained by coarse-graining the electronic structure while preserving the quantum-mechanical nature of the chemical bond. The analytic BOP allows 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.

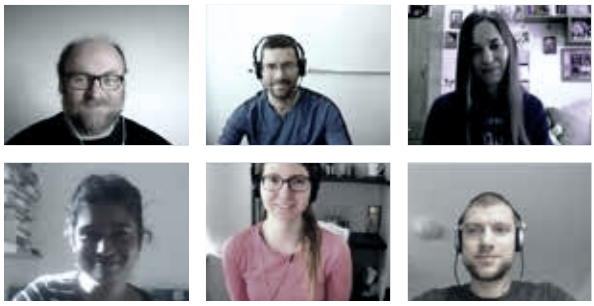


Fig. 4.3: Video call of the group in 2021.

▸ 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 with domain knowledge of the interatomic interaction
- Structural stability, point defects and interfaces in transition metal compounds

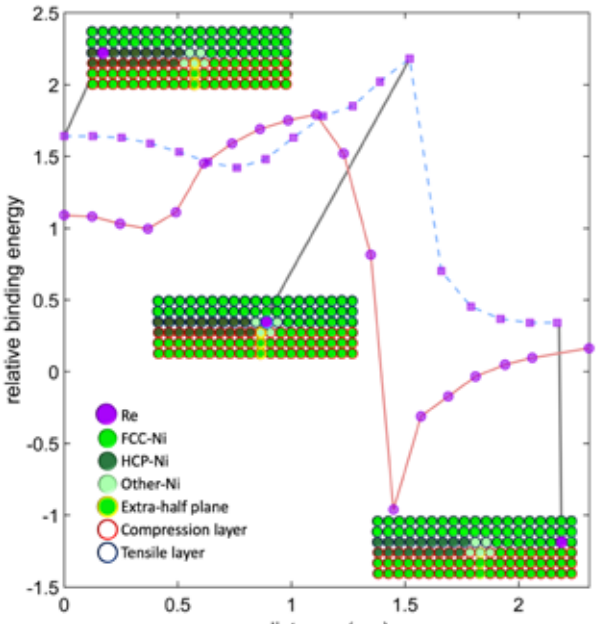


Fig. 4.4: Relative binding energy of Re at a stacking fault in Ni as a function of the distance to the centre of the stacking fault in the tensile (squares, light blue line) and compressive layers (disks, light red line). (New J. Phys. 21 (2019) 123020)

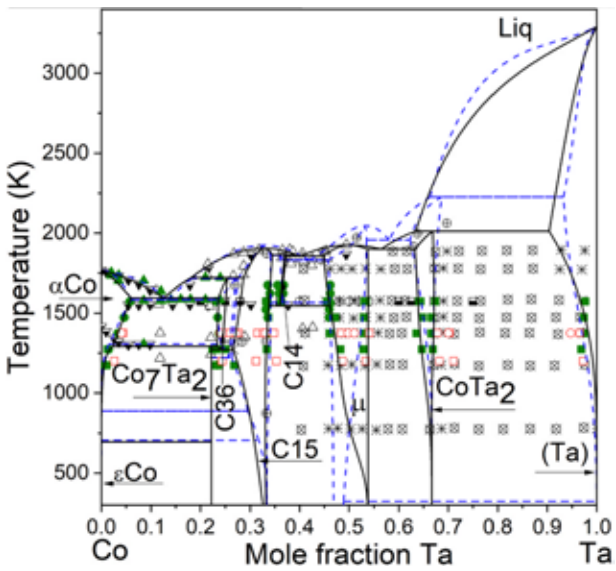


Fig. 4.5: Phase diagram of Co-Ta, obtained on the basis of density-functional theory calculations for ordered bcc, fcc, hcp, C_{14}, C_{15}, C_{36}, mu, and C_{16} crystal structures and available experimental data (symbols). (CALPHAD, 64 (2012) 205)

4.2. Atomistic Simulation of Mechanical Behaviour

Group leader:
Dr. Matous Mrovec

Group members:
Dr. Antoine André Maroun Kraych
Minaam Qamar
Matteo Rinaldi
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 the modelling of intrinsic material properties related to chemical bonding but eventually concentrate on the role of crystal imperfections. The imperfections encompass fundamental crystal defects, such as vacancies, dislocations and grain boundaries in single-component crystalline materials as well as complex microstructural features such as semi-coherent interfaces, precipitates and secondary phases that constitute the microstructure of technologically important multi-phase and multi-component systems.

The materials we are interested in include those with prototypical metallic and covalent chemical bonding 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 novel interatomic potentials. Recently, we have focused on the development and application of atomic cluster expansion (ACE) models which can reach the accuracy and transferability of electronic structure methods while remaining highly computationally efficient and applicable in large-scale atomistic simulations. We also integrate the atomistic simulations with mesoscale techniques (DDD, kMC), phenomenological and continuum theories as well as experiments.

▸ Competences

- Interatomic potentials
- Transition metals and their compounds
- Crystal defects and imperfections
- Hydrogen embrittlement
- Magnetism

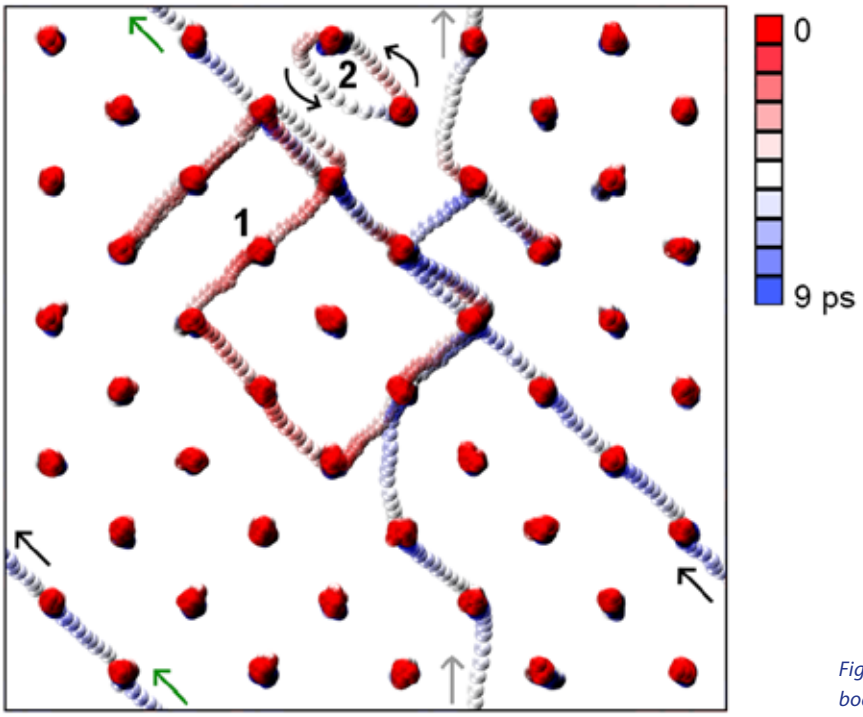


Fig. 4.6: Concerted migration of atoms in body-centered cubic Ti at 1800 K.

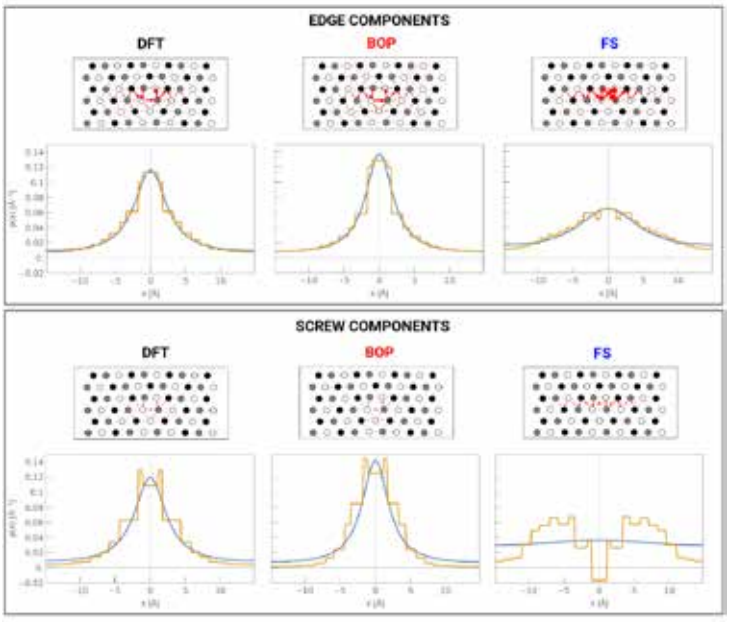


Fig. 4.7: Cores of mixed M111 dislocations in W predicted by different atomistic models.

AMS

4. 3. Data-Driven Methods for Atomistic Simulations

Group leader:
Dr. Yury Lysogorskiy

Group members:
Dr. Anton Bochkarev
Sarath Menon

▸ Research

The research group is working on the development and application of data-driven methods in materials science with a particular focus on the atomic scale. This includes the development of the Atomic Cluster Expansion (ACE) – a new class of many-body interatomic potentials – starting from code development to fitting of new potentials and their validation. For this we utilize modern computational technologies and concepts, such as GPU computing.

Our second major research area is the automated 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 for Iron Research.

Another research area is the application of general data-driven modeling to materials science in a collaboration with the Materials Discovery and Interfaces group, for example, predicting structure zone diagrams for thin-film synthesis by generative machine learning.

▸ Competences

- Atomic Cluster Expansion: development and validation
- Validation of interatomic potentials (atomistictools.org)
- High-throughput calculations (DFT and molecular dynamics)
- Data-driven methods in materials science: machine learning, generative models

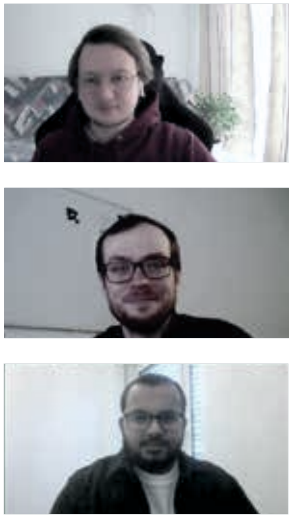


Fig. 4.8: Video call of the group in 2021.

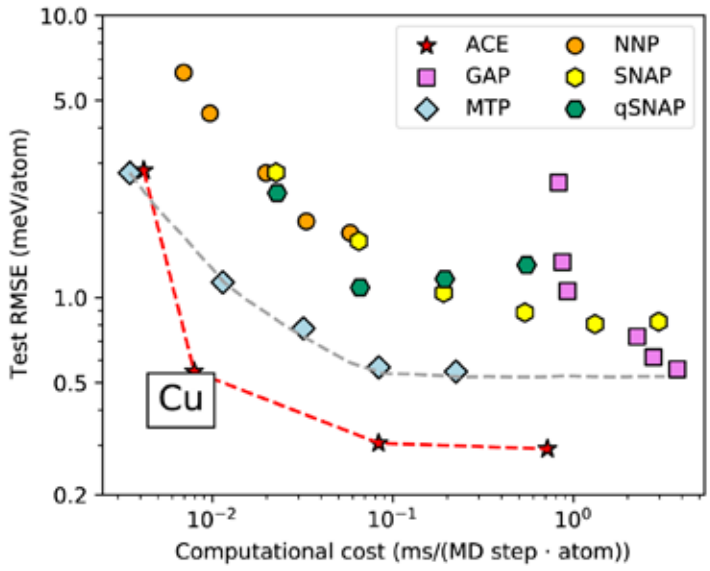


Fig. 4.9: Test error versus computational cost for Cu ACE potential compared to a recent benchmark study of machine learning interatomic potentials. The timings of ML potentials were reduced by constant factors 0.55 to correct hardware differences and the new ACE timings then overlaid.

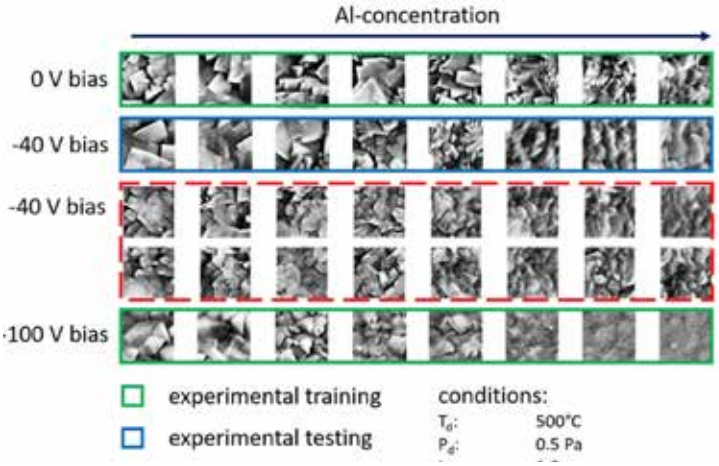


Fig. 4.10: cGAN predictions for the effect of bias voltage (EI) and Al concentration on the surface microstructure (red dashed box) vs. images from the experimental test set (blue box). The green boxes show images from the experimental training set. [image is taken from I. Banko, Y. Lysogorskiy et al. Commun Mater 1, 15 (2020)]

ICAMS

Department Scalebridging Thermodynamic and Kinetic Simulation STKS

5. Department Scalebridging Thermodynamic and Kinetic Simulation

Prof. Dr. Ingo Steinbach

▸ Research

The department focusses on the processing of materials: The evaluation of materials microstructures from solidification through thermomechanical processing and, in a generalized sense, during service until failure. Materials microstructures determine their properties, and they are by far not static.

In a scale-bridging approach we incorporate atomistic methods to develop predictive constitutive models at the mesoscopic scale. These are used to predict macroscopic materials properties dependent on the actual state of the microstructure. Among the numerical techniques applied within our department are first-principles methods for phase-stabilities, the CALPHAD method (CALculation of PHAse Diagrams) to calculate phase-stability, molecular dynamics to determine interface properties, 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. In addition, finite element methods are used, e.g., to predict damage processes in biological tissues. A new research line opened by Dr. Julia Kundin centeres around "Diffusion in Metals and Minerals".

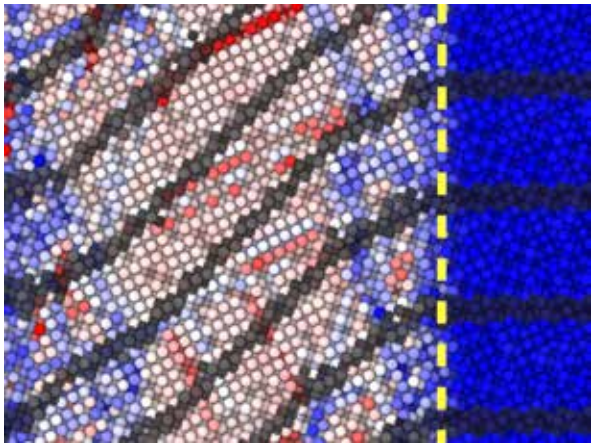


Fig. 5.1: MD simulation of coupled motion of a random grain boundary in aluminium (A. Schratt, V. Mohles, Comp. Mater. Sci. 182 (2020) 109774).

▸ Structure

- The department's activities are organized in four groups focusing on different materials and techniques.
- 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)
- Diffusion in Metals and Minerals (Dr. Julia Kundin)

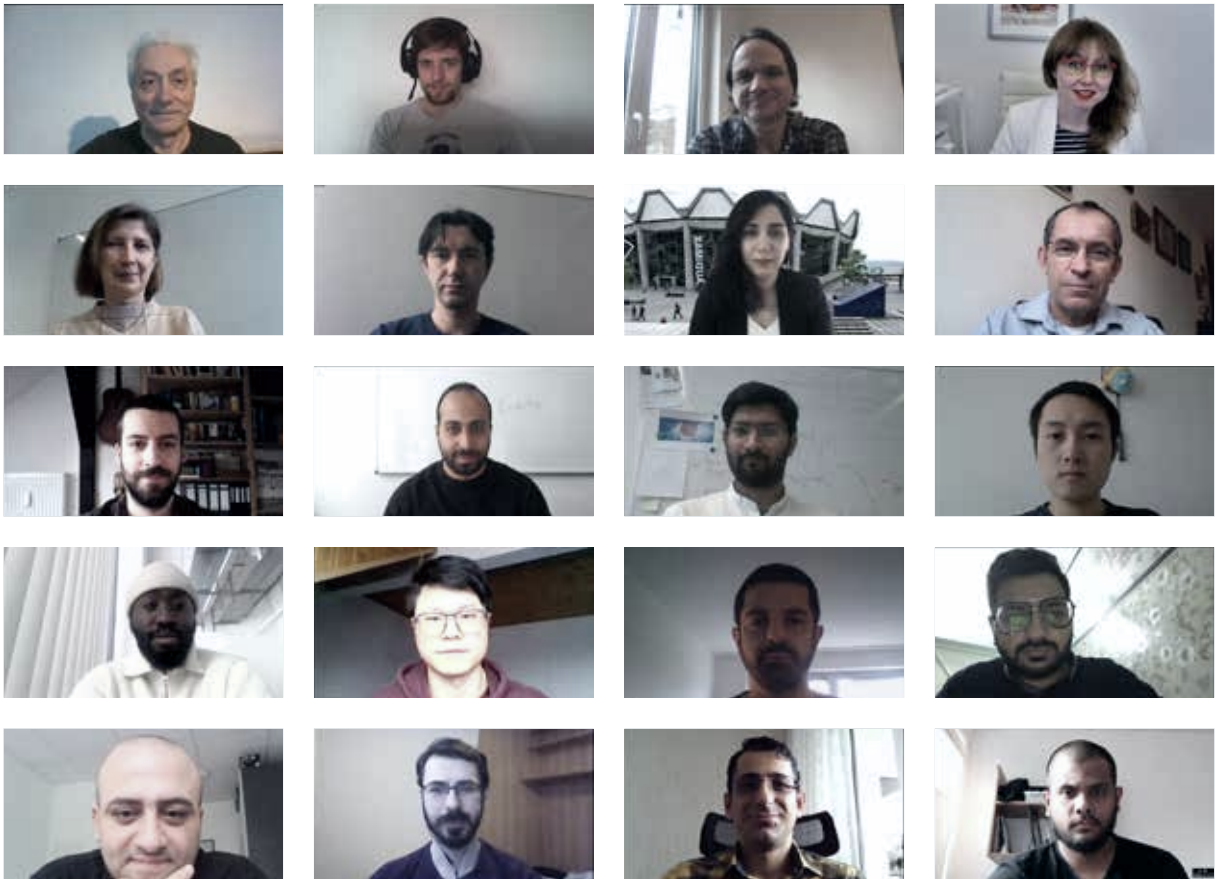


Fig. 5.2: Video Conference of the STKS department.

STKS

5.1. Phase-Field Simulation of Microstructures

Group leader:
Dr. Oleg Shchyglo

Group members:
Muhammad Adil Ali
Stephan Hubig
Hesham Salama
Murali Uddagiri

► Research

Our research group focuses on the development of new methods for phase-field simulations of microstructures in complex materials. At present, the range of applications for phase-field modelling includes solidification that is controlled by the solute and heat diffusion, grain growth in systems with strong anisotropy of their interface properties, eutectic and peritectic reactions in multicomponent systems, static and dynamic recrystallization, martensitic and bainitic transformations in steel, modelling of superalloy microstructure formation and its stability at in-service conditions. Aiming to make a quantitative prediction of the microstructure formation in these processes, 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 plasticity 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 consider the free energy contributions which are at present omitted in the thermodynamic databases. Combining the micromechanics and thermodynamics by using our in-house expertise in both fields, we aim to further advance the understanding of microstructure formation mechanisms in martensitic and bainitic steels as well as the microstructure stability of superalloys at in-service conditions.

► Competences

- Phase-field modeling
- Phase transformations
- Microscopic elasticity theory
- "OpenPhase" library development

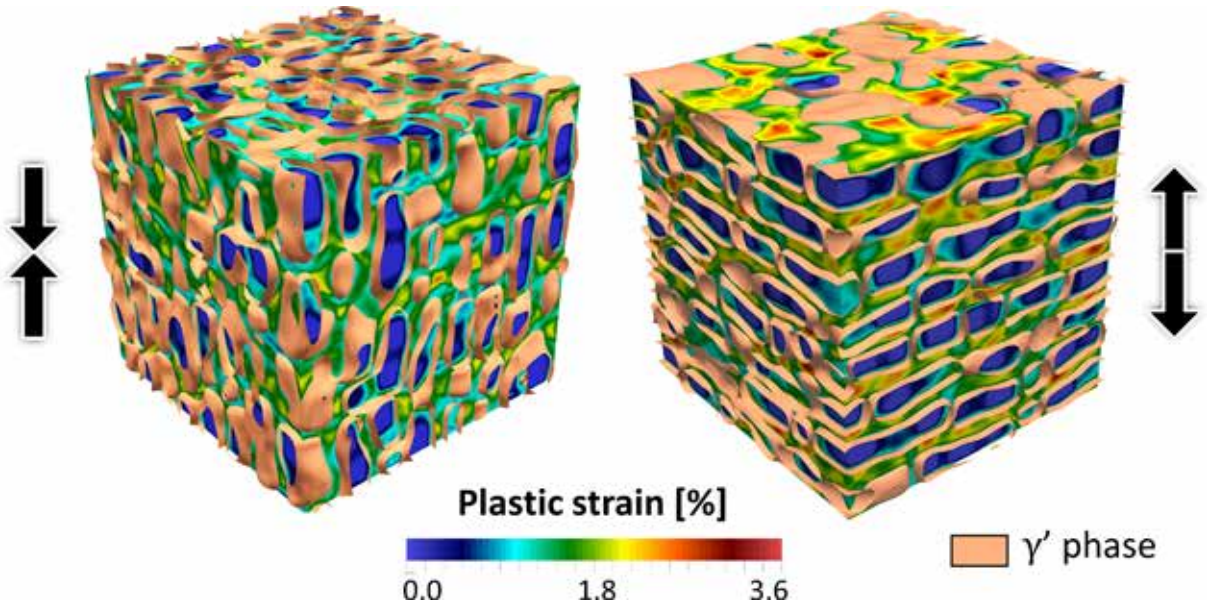


Fig. 5.3: High tempewrature low stress creep simulations of Ni-based superalloys under compression (left) and tension (right)..

5.2. Theory and Simulation of Complex Fluids

Group leader:
Prof. Dr. Fathollah Varnik

Group members:
Marian Bruns
Haifeng Wang
Dr. Elias M. Zirdehi

▸ Research

Research interests of the group cover a broad range of physical phenomena including mechanical response and structural relaxation in polymers, microstructure evolution in metallic foams, and effects of thermal history on mechanical properties of amorphous solids.

Recently, a particular focus of the complex fluids group has been on the effect of small additive molecules on shape-memory behavior in polymers. It has been shown via extensive molecular dynamics simulations that small molecules enhance the dynamics of structural relaxation in the polymer matrix and thus lead to the onset of shape recovery at a lower temperature as compared to a pure sample. This finding has strong implications on the application side as additive molecules may be used to tune the triggering temperature for the shape recovery process.

Another recent activity within the group has been modelling metallic foam on the mesoscale. This is a multi-physics problem, which includes phase transformation and microstructure evolution in liquid-gas systems containing chemical agents, which serve to hinder coalescence of adjacent bubbles during the experimentally relevant time window. The model is based on a combination of the multi-phase-field model with a solver for fluid dynamic equations.

In addition, the group investigates effects of cyclic thermal treatment between temperatures well below and well above the glass transition temperature (known as cryogenic cycling) on mechanical properties of metallic glasses. Here, the underlying idea is that the structure of glassy systems is usually heterogeneous on some small length scales, the latter depending on the material as well as the production process. Via molecular dynamics simulations, the question is addressed whether and how cyclic thermal treatment and the resulting thermal expansion and contraction improve ductility of metallic glasses.

▸ Competences

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

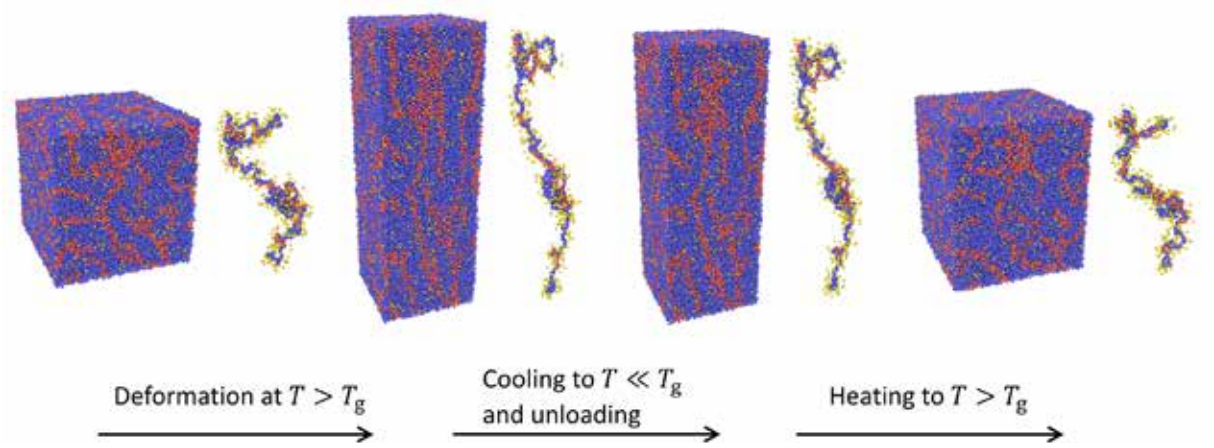


*Fig. 5.4: Molecular dynamics simulation result of a shape-memory cycle using a bead-spring copolymer model. The sample first deformed at a temperature above its glass transition, T_g. Then it is cooled to a temperature below T_g. At the end of the cooling procedure, it is unloaded. The sample first deforms back slightly due to its energetic elasticity, but the major part of deformation is stored as it is connected to entropic elasticity, the latter becoming active at temperatures above the glass transition. Therefore, shape recovery takes place only if the sample is heated to a temperature $T > T_g$. Image from Zirdehi et al, Materials **10**, 14(2):327 (2021).*

5.3. Data Mining and Statistical Analysis

Group leader:
Dr. Irina Roslyakova

Group members:
Abdulmonem Obaied
Setareh Zomorodpoosh

▸ Research

The group focuses on developing multi-scale modelling and design approaches to produce reliable and robust new materials. This is achieved by combining artificial intelligence, data mining, and physics-based modeling, with synthetic materials that are artificially generated by computer simulations, to provide novel alternative solutions based on existing theoretical model predictions. This Artificial Material Intelligence (AMI) approach is able to predict mechanical properties for complex and microstructure-dominated materials and to accelerate the discovery of new materials data. One of the group's main research topics is the study of the thermodynamic, microstructural and mechanical properties of single-crystal Ni- and Co-based superalloys using physically sound statistical models and high-throughput machine learning algorithms. Such an approach made it possible to study the relative microstructure properties of Ni- and Co-based superalloys using a state-of-the-art image mining algorithm. In comparison to the existing manual method, such a modelling method results in a faster, more consistent and more efficient analysis of different types of data (tabulated or graphical). In addition, combining this modelling approach with the statistical application of design of experiments reduces the number of experimental trials required for the development of new materials and processes.

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

- Development of physics-based data-driven modeling strategies for accurate and robust description of thermodynamic and mechanical material properties.
- Application of materials informatics including image analysis by computer vision to support computer-based design of new nickel- and cobalt-based superalloys.
- Design and implementation of well-organized data infrastructure for storage, management, and automated processing of experimental data and simulation results, in particular, creep experiments, including SEM/TEM images of microstructures and associated metadata.
- Development and application of data mining and machine learning methods to identify statistically sound correlations between materials chemistry, microstructure, and mechanical data.

▸ Competences

- Material informatics including data and image mining and machine learning methods
- Automation of data and image processing on different scales
- Automation of partial aspects of kinetic and thermodynamic CALPHAD-type re-assessments using statistical and machine learning

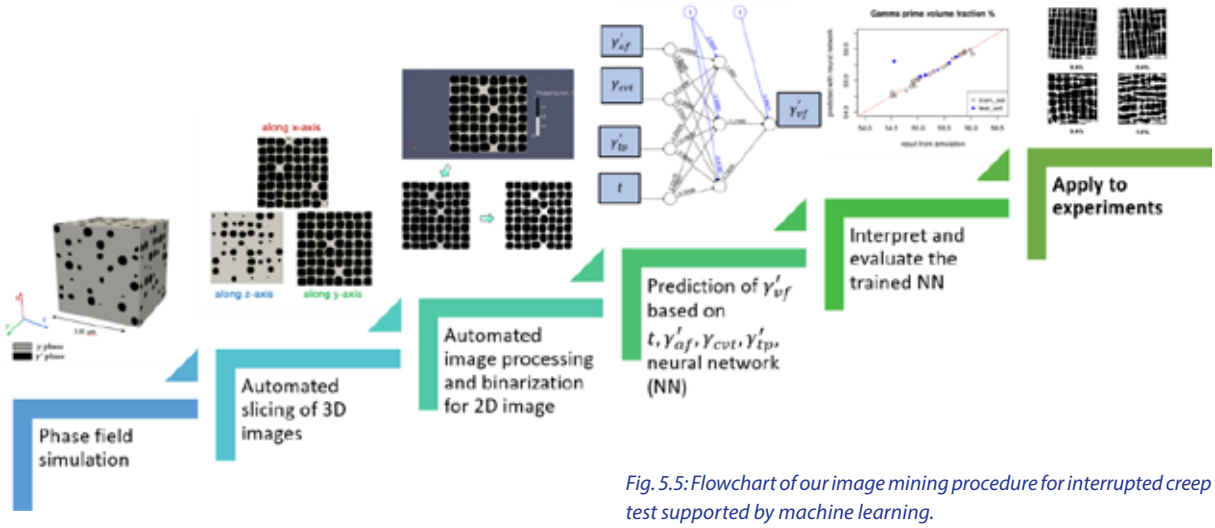
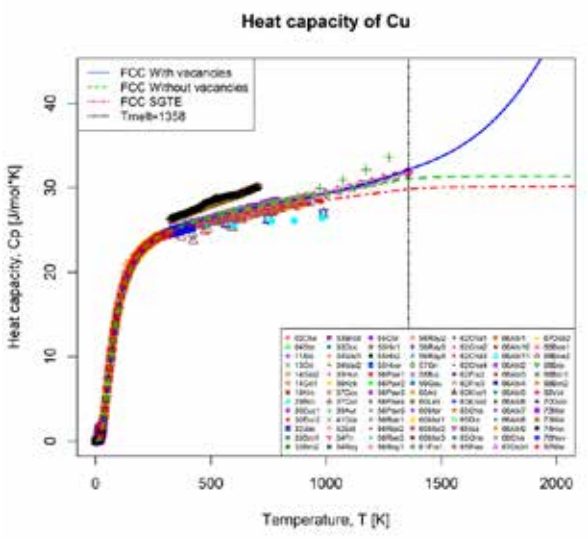


Fig. 5.5: Flowchart of our image mining procedure for interrupted creep test supported by machine learning.

Fig. 5.6: Modelling thermal vacancies explicitly in the frame of the third generation CALPHAD database from 0K using segmented regression model: example of pure Cu.



- Development of physics-based materials properties models
- Development of the third generation CALPHAD databases from 0 K, in particular, mathematical aspects of physics-based modeling of the thermophysical properties and their application for CALPHAD-type re-assessment of binary and high order systems.

ICAMS

Department Micromechanical and Macroscopic Modelling MMM

MMM

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 investigate microstructure-property relationships by employing the methods of computational materials science and multiscale modelling, aiming to achieve an understanding of fundamental deformation and failure mechanisms and also to predict macroscopic mechanical properties of materials, like strength under monotonous and cyclic loading, hardness, and fracture toughness. A new direction of our work, which has been rapidly gaining importance, is the branch of data-oriented materials science, in which the powerful tools of machine learning (ML) are applied to find correlations in various kinds of data on the mechanical performance of materials. In this respect, the physics-based models developed in our group are well-suited to produce the large amounts of data that are necessary to train machine learning algorithms to mimic real material behavior.

With this work in the field of data-oriented materials science, we were able to produce a proof of concept showing that ML algorithms can in fact be trained with data from micromechanical models. Such data can be obtained from a representative volume element (RVE) of a given microstructure, as demonstrated in the calculation of stress-strain curves for a polycrystal with a Goss texture under different loading directions (*Fig. 6.1*). In the data-oriented approach, the trained ML algorithms are used as constitutive models that describe the mechanical behavior of a material on the macroscopic level. It is seen that the performance of the ML models is quantitatively comparable to standard constitutive models (*Fig. 6.2*), however, with the advantage that microstructural information is seamlessly integrated into the ML concept. In other words, ML constitutive models bridge the scales from the microstructure to the component level by introducing numerically efficient material models that implicitly contain microstructure-property-relationships.

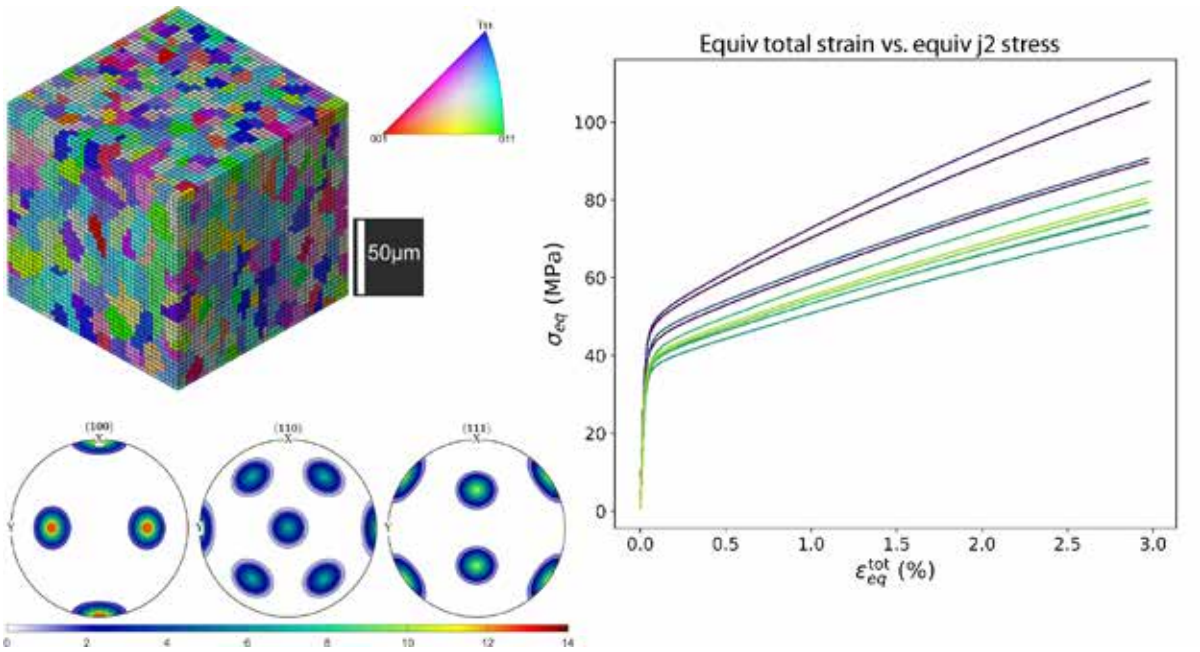


Fig. 6.1: A representative volume element (RVE, upper left) of a polycrystal with a Goss texture as given by the orientation distribution function (lower left) is characterized with respect to its stress-strain-behavior under different loading directions (right). The loading directions are indicated by different colors of the stress-strain curves. The mechanical behavior of the polycrystal is described with the crystal plasticity finite element method (CP-FEM).

The research activities on fatigue properties of metals were very fruitful in the past years, having produced plenty of insight into the mechanisms of cyclic plasticity and damage evolution under cyclic loading conditions. Based on realistic representations of microstructures and rather fundamental crystal plasticity (CP) models, the influence of microstructure on the fatigue strength and lifetime of various materials, like martensitic and austenitic steels as well as nickel-based superalloys, has been investigated; see (*Fig. 6.3*) for an example on martensitic steel. Furthermore, a novel inverse method has been devised that allows the identification of the parameters for cyclic plasticity from quasi-non-destructive cyclic indentation experiments (Sajjad et al. Materials 13(2020)3126, https://doi.org/10.3390/ma13143126).

The research activities on modeling of interfacial properties and realistic microstructures are described in the following sections. The department MMM is currently organized into the three research groups "Mechanical Properties of Interfaces" (Rebecca Janisch) and "Micromechanics of Large Deformations" (Napat Vajragupta), and "Discrete Micromechanics and Fracture" that has been led by Alexander Hartmaier, after Dr.-Ing. Hamad ul Hassan left ICAMS in January 2020. We sincerely thank Dr. Hassan for his important contributions to the research at ICAMS in the field of fracture and fatigue. The focus of this research group will gradually shift into the direction of data-oriented materials science with applications on plastic deformation and failure, while the successful work on fatigue modelling will be continued. The data-based research activities are conducted in close collaboration with the department "Materials Informatics and Data Science" headed by Prof. Markus Stricker.

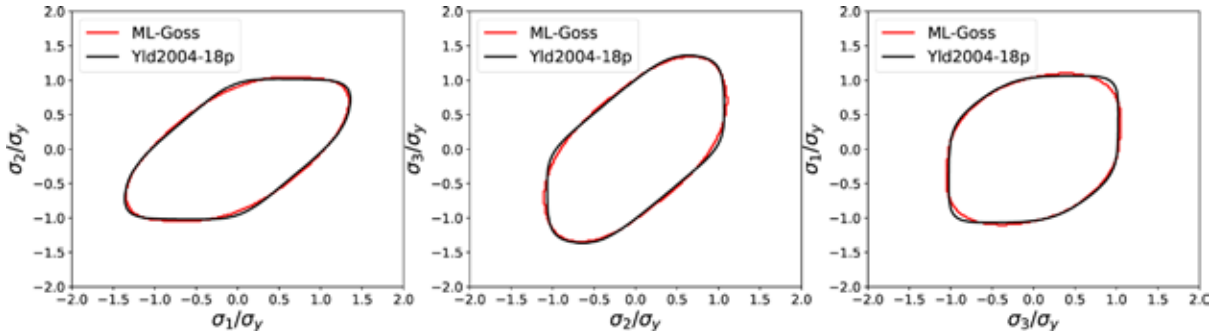


Fig. 6.2: Yield surface of a polycrystal with a Goss texture, displayed as slices through the principal stress space. The results obtained from the ML constitutive model and the 18-parameter Barlat model (Yld2004-18p) fitted to the same data are compared.

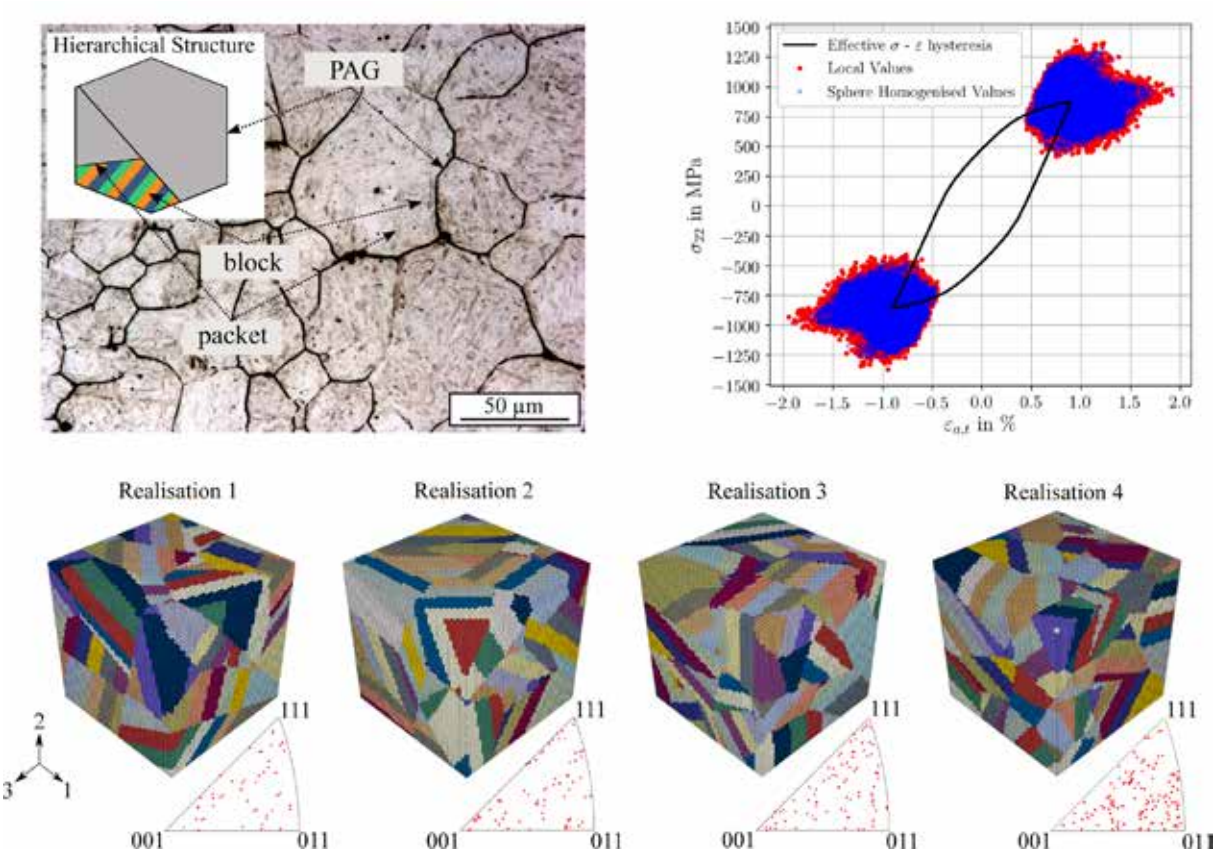


Fig. 6.3: The hierarchical microstructure of the martensitic steel SAE 4150 is analyzed (top left), and different realizations of a small RVE capturing the microstructural features in a statistical sense are generated (bottom). The mechanical behavior of these RVE under cyclic loads is analyzed with CP-FEM, which reveals not only the macroscopic stress-strain hysteresis, but also provides insight into the evolution of local stresses and strains within the microstructure (top right) (see Schäfer et al. Materials 12(2019)2825, https://doi.org/10.3390/ma12182852).

MMM

6.1. Mechanical Properties of Interfaces

Group leader:
Dr. Rebecca Janisch

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

► Research

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

Ab-initio electronic structure calculations based on density functional theory are used to predict the energy, strength, and effective modulus of interfaces and other defects in iron and ferritic steel. These characteristic properties are used to identify and understand trends, e.g. on hydrogen solubility in ferritic microstructures and on its effect on grain boundary cohesion. Thus, guidelines for alloy design and constitutive relationships for multiscale simulations, e.g. of hydrogen enhanced decohesion, are derived.

Via large scale atomistic simulations the fundamental deformation and crack propagation mechanisms in interface-dominated microstructures are determined – such as interfacial sliding, migration, dislocation emission, and twinning in fully lamellar TiAl alloys – and are related to fundamental physical quantities, such as surface and stacking fault energies.

In 2019/2020 the projects of the group focused on the role of H in the competition between inter- and transgranular fracture in ferritic steel, and the processes at semi-coherent interfaces in lamellar TiAl during deformation and fracture. Among the main insights were that bulk cleavage planes in Fe are much more sensitive to H effects (such as hydrogen-enhanced decohesion) than special grain boundaries, and that the consideration of semicoherent interfaces is crucial to understand the difference between volume fraction and size effects in two-phase lamellar TiAl.

Fig. 6.4: Group Photo in 2020.

► Competences

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

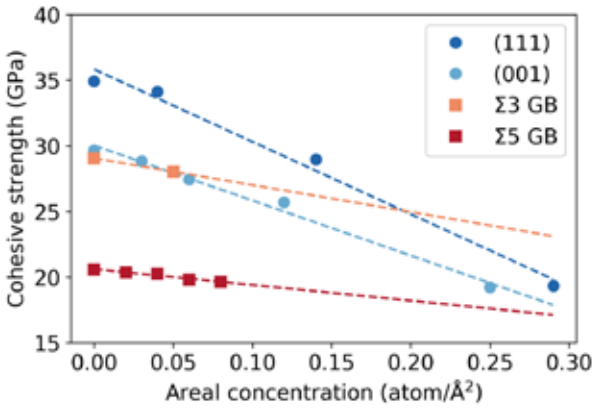


Fig. 6.5: Influence of H on the cohesive strength of (111) and (001) bulk cleavage planes as well as two different symmetrical tilt grain boundaries in bcc Fe. The results were obtained by ab-initio density functional theory calculations, See Guzmán et al., Materials 13 (2020) 5785.

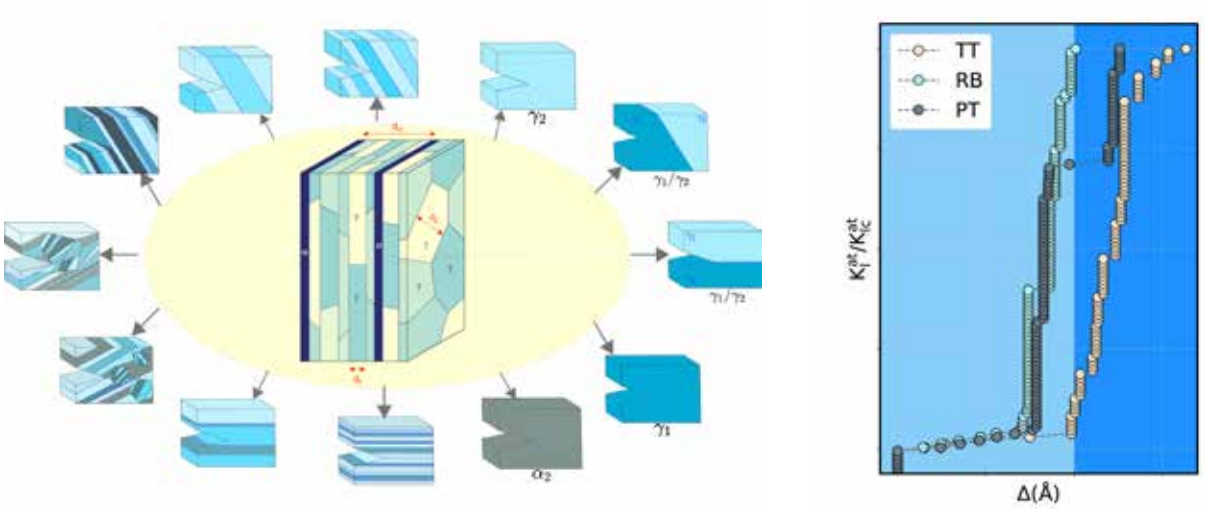


Fig. 6.6: Schematics of different set-ups to study fracture in two-phase lamellar Ti-Al alloys via large-scale molecular dynamics simulations and crack resistance curves that result from such simulations.

MMM

6.2. Micromechanics of Large Deformations

Group leader:
Dr.-Ing. Napat Vajragupta

Group members:
Abhishek Biswas
Shengli Li

► Research

The research group Micromechanics of Large Deformations aims at using micromechanical modelling to describe deformation mechanisms of materials or components. To achieve this goal, we focus on four research areas, microstructure digitalization, crystal plasticity models, parameterization of material models by inverse methods, and in-depth analysis of microstructural deformation mechanisms.

The method for digitalizing microstructures is of crucial importance because it must capture all important microstructural features. We aim to provide an easy-to-use solution for digitalizing microstructures, which is applicable for existing materials and capable of creating synthetic microstructures with desired features.

As new materials are continuously being developed, more advanced models are required to describe complex deformation mechanisms. Thus, we continuously intensify our expertise in crystal plasticity. The formulation and application of inverse methods to parameterize material models are also within the scope of our work.

The combination of digitalized microstructures and parameterized material models allows us to gain insight into the dependence of deformation mechanisms on microstructural features. In 2019/2020, our research group was active in developing the open-source synthetic microstructure generator Kanapy, which is capable of reproducing real grain geometries and crystallographic textures in a statistical sense, in parameterizing a non-local crystal plasticity model using nanoindentation, and in micromechanical modeling of additively manufactured metals.

Fig 6.7 provides the workflow for creating a synthetic microstructure of an existing material by using Kanapy. From the EBSD map, the orientation distribution function (ODF)-reconstruction module discretizes a given ODF into a set of crystallographic orientations. In parallel, the geometry module analyzes the grain geometry and creates a microstructure model that mimics the real grain geometry. The crystallographic orientation set is assigned to this microstructure model while also considering the real misorientation distribution function, which result in a synthetic microstructure that represents the real one in a statistical sense. *Fig. 6.8* shows the influence of pore characteristics on the anisotropic mechanical behavior studied by micromechanical modelling. The shape of pores affects the anisotropy in the mechanical behavior. Elongated pores promote pore coalescence during loading in transverse direction at smaller equivalent plastic strains than for loading in the building direction, which signifies the anisotropy in the strength due to the pore shape.

► Competences

- Microstructure digitalisation
- Microstructure characterisation and analysis
- Crystal plasticity modelling
- Parameterisation of material models by inverse methods
- Model-based identification of microstructural deformation mechanisms

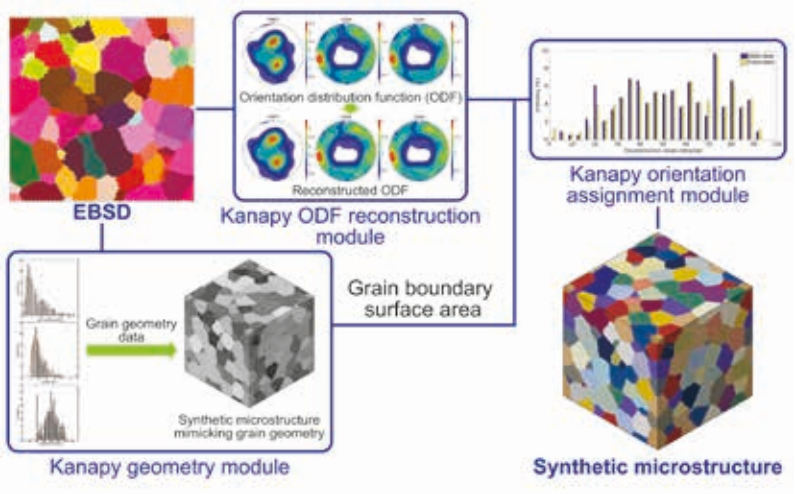


Fig. 6.7: The workflow for creating a synthetic microstructure of an existing material using Kanapy. See Prasad et al. J. Open Source Softw. 4 (2019) 1732.

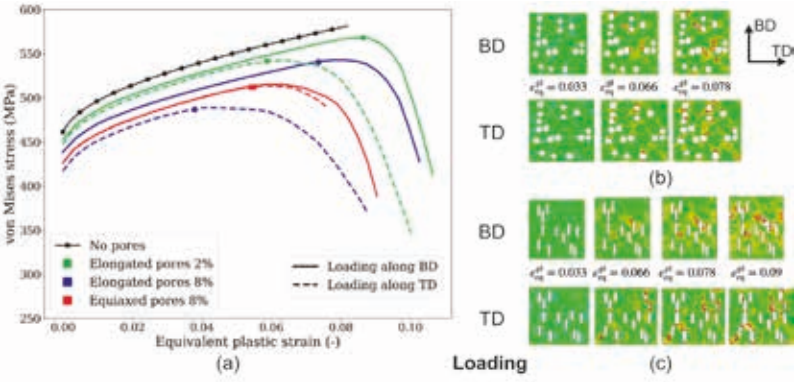


Fig. 6.8: Influence of pore characteristics on anisotropic mechanical behavior revealed by micromechanical modeling. (a) Comparison of stress-strain-curves for different pore shapes, pore coalescence, showed using 2D cross-sectional views of deformed micromechanical models with (b) equiaxed pores and (c) elongated pores loaded along the building (BD) and transverse (TD) directions. See Prasad et al. Adv. Eng. Mater. 22 (2020) 2000641.

ICAMS

High-Performance Computing in Materials Science

HPC

7. High-Performance Computing Materials Science

Group leader:
Prof. Dr. Godehard Sutmann

Group members:
Stephan Schulz

▸ Research

The research group High -Performance Computing in Materials Science 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 linking to the other ICAMS departments and supports the development of simulation codes and efficient parallelization of programs, developed at ICAMS and international communities. Currently, one focus is given to new approaches of continuum mechanics modeling for plastic deformation, coupled Monte Carlo and Molecular Mechanics simulations and efficient ways to balance the computational work on large parallel clusters. These works are linked in part to the other ICAMS departments. Research and development is performed in close cooperation with the Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich and the CECAM community.

The Euler-Lagrange particle-based Materials Point Method (MPM) has been implemented into a new code and is further developed to simulate materials in the continuum description. In contrast to established methods, such as the Finite-Element-Method (FEM), it shows great adaptability to large deformations since the material is represented by particles which are suitable to adapt geometrically to deformations without any need for remeshing. The interaction between particles is computed on a regular grid after transferring the necessary properties from the particles, which both increases performance for computations and provides a basis for an efficient parallelization. Therefore, the work on the MPM code also considers an efficient parallelization, which is done in cooperation with the Jülich Supercomputing Centre. The work further includes substantial improvements of boundary conditions in MPM, which have been considered in analogy to electrostatic image particles and which allows to implement consistent no-slip boundary conditions.

The code has been tested for a crystal plasticity model and has been applied to an equi-channel angular pressing (ECAP) set-up (*Fig. 7.1*). To support such simulations, the generation of suitable geometry inputs was added as well as the corresponding support of arbitrary material shapes. Since the image particle method prohibits any movement perpendicular to a boundary, material tends to stick to boundaries even when moving only away from it. So the method was extended to the oriented image particle method, which only applies the boundary condition if the particle moves towards a given boundary, allowing the material to cleanly separate from walls.

Since efficiency of parallel simulations depends on the well-balanced partitioning of work, load balan-

cing has been taken into account for the MPM code. This has been realized by a common initiative with Jülich Supercomputing Centre to extend a load balancing library, originally developed at JSC. It has been extended to a Fortran interface and the ability to consider also domain decompositions including discrete length scales, as it often appears in cell-based algorithms for particle-based simulations. This also allows for efficient dynamic partitioning of meshes. The basic algorithm has been chosen as a staggered mesh, which allows, in principle, an exact partitioning for appropriate work functions (*Fig. 7.2*). Remaining scatter around the average value of runtime results from differences in runtime behavior of processors, neglect of communication times in the balancing, minimum width of domains in cartesian directions and discrete shift of domain boundaries implied the computational mesh.

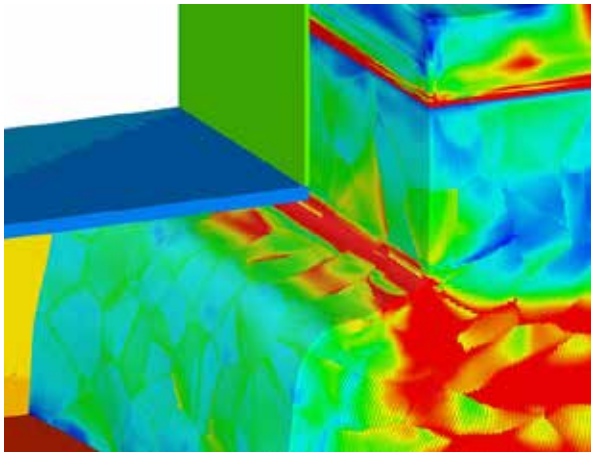


Fig. 7.1: Detailed view of the equi-channel angular pressing (ECAP) simulation of a polycrystalline system.

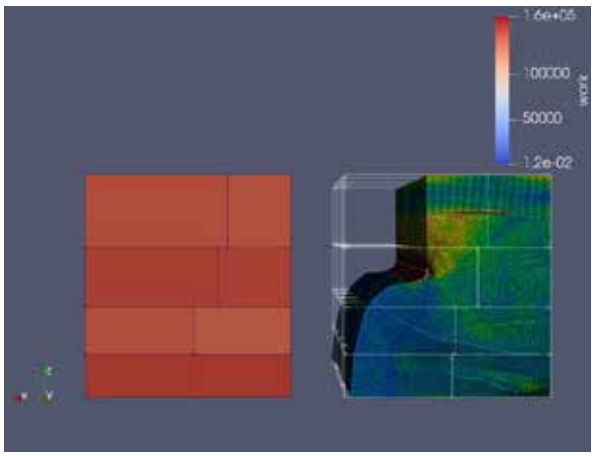


Fig. 7.2: Time-dependent load balancing and adjustment of domain geometries during a dynamic ECAP simulation, to improve parallel efficiency.

For systems where the computational load is time-independent, a static load balancing scheme, based on partition functions, has been developed, which allows for domain partitioning on an arbitrary number of processers. A fast partitioning method has been developed based on a hierarchical implementation of integration, which can be applied for staggered meshes, best surface-to-volume decompositions or alternating orthogonal recursive bisections. The new method has been tested for the large-scale Lattice-Boltzmann code HemeLB on thousands of processors.

Applications on new parallel architectures require a certain degree of code flexibility and adaptability due to the fast evolution of programming architectures and paradigms. The framework Kokkos, which maps data structures in an efficient way on different architectures, offers performance portability between different HPC platforms. Kokkos has been applied to an electrostatics solver, based on the Ewald summation method and has been shown to keep performance when being ported from a CPU-based Intel cluster to an Nvidia- or AMD-based GPU cluster.

The simulation of segregation of interstitial atoms in metals has been considered by a coupled Monte Carlo and Molecular Statics method. Parallelization is realized via a Manager-Worker approach. A strong efficiency drop was observed when the system segregated, e.g. close to a dislocation, and density concentrations had locally increased. To overcome this efficiency drop a biased Monte Carlo method has been developed, which profits from the consideration of the evolution of density inhomogeneities and from taking into account regions in configuration space with both higher and lower acceptance probabilities of particle moves in the Monte Carlo protocol. The method proved much more efficient to segregate particles (*Fig. 7.3*) towards perturbations, e.g. single dislocations or dislocation networks.

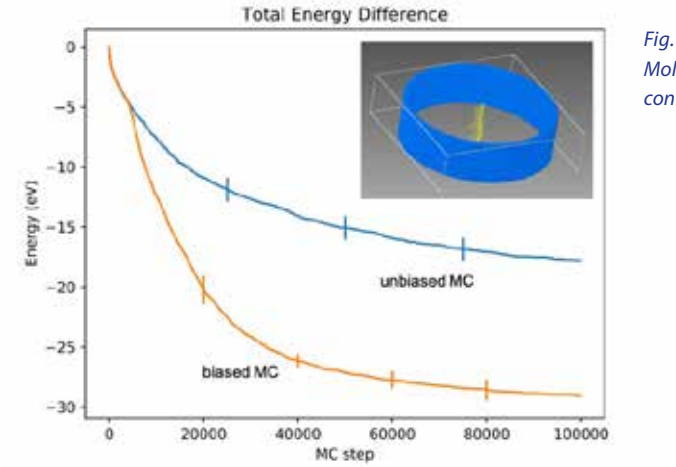


Fig. 7.3: Comparison of system energy during hybrid Monte Carlo/ Molecular Statics simulations using unbiased and biased sampling of configuration space in a Fe-C system.

ICAMS

Scale-Bridging Simulation of Functional Composites SFC

8. Scale-Bridging Simulation of Functional Composites

Group leader:
Prof. Dr. Anna Grünebohm

Group members:
Aris Dimou
Dr. Ruben Khachaturyan
Sheng-Han Teng

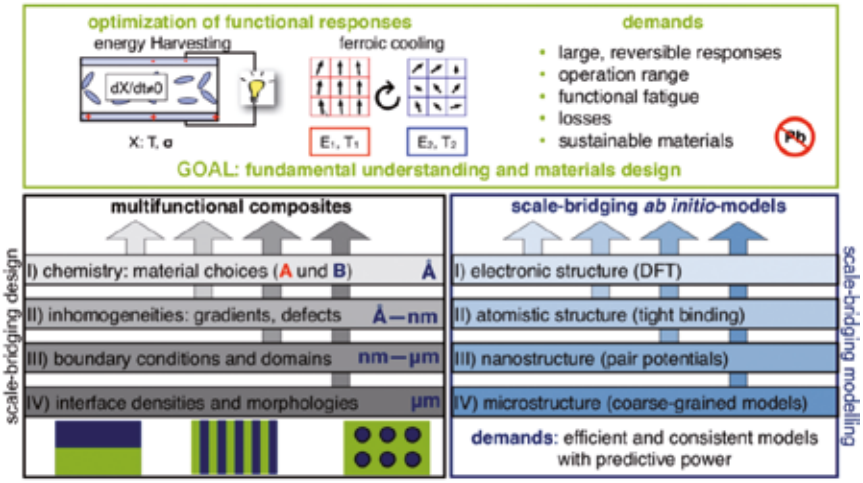
▸ Research

Ferroelectric perovskites (ABO3, with A: alkali earth metals and B: transition metals) are widely used in applications and are promising for energy harvesting devices as well as for future efficient solid-state cooling devices based on the electrocaloric effect. All these applications share the following demands on materials design: Replace problematic elements and increase efficiency and reversibility in a broad and suitable operation range.
The goal of the group is the design of ferroic materials and composites with superior functional properties. Our approach is the scale-bridging optimization of microstructures and composite morphologies, combining the benefits of materials choice, controlled inhomogeneities, domain engineering and interface design.
Our methods are scale-bridging simulations based on ab initio parametrization with high predictive power, which allow us to fundamentally understand and design the properties of materials systems

▸ Competences

- Molecular dynamics simulations
- Density functional theory
- Ferroic materials and composites
- Functional (piezoelectric, dielectric, caloric) responses.

In 2019/2020 the group focused on the coupling between strain and microstructure (domains) and the impact of domains, substitution and atomic ordering on ferroic switching, and phase transitions in $BaTiO_3$.



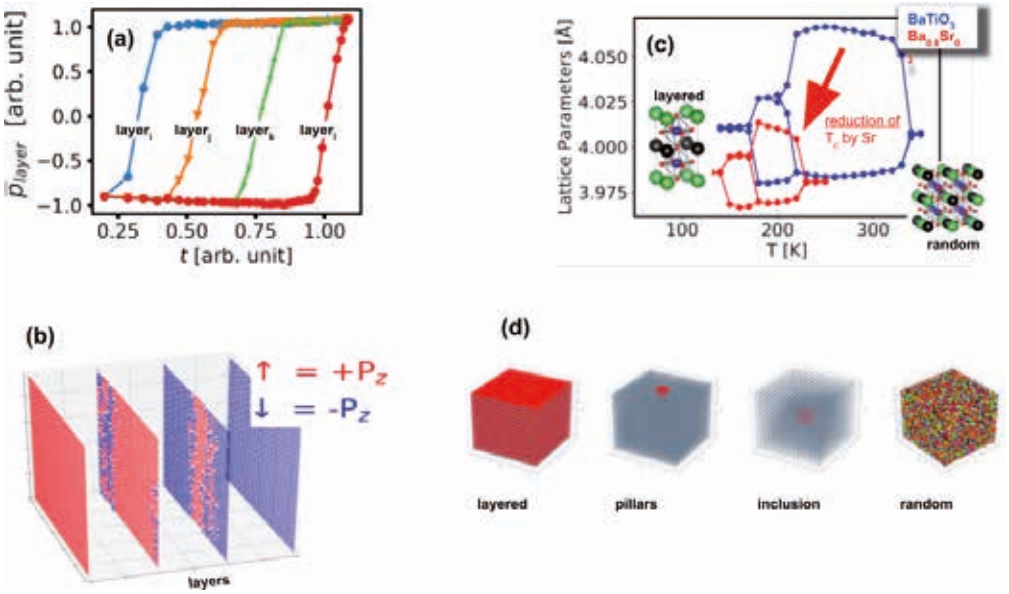


Fig. 8.1: Scale-bridging simulation of domain walls and inhomogeneities in (Ba,Sr)TiO_3: (a)—(b) Local polarization and switching kinetics in the presence of 180° domain walls. (a) The wall propagates through the system and switches polarization in successive layers by nucleation and growth on the wall as shown in (b).
(c) For a homogenous distribution of substituents, the main impact of Sr is a reduction of transition temperatures. Different local atomic ordering (insets) modify subtle details and nano-scale inhomogeneities (d) turn the material properties inside out.

ICAMS

Materials Informatics and Data Sciences

9. Materials Informatics and Data Sciences

Group leader:
Prof. Dr.-Ing. Markus Stricker

▸ Research

The research group "Materials Informatics and Data Sciences" is currently being established. The corresponding new junior professorship representing the field "Data-Driven Materials Research" was awarded in July 2020. Key elements of the new research group are the application of statistical and machine learning methods as well as data science approaches to materials science problems mostly based on simulated data. With this focus the new research group strengthens and extends the informatics activities at ICAMS. Applications of these methods focus on bridging between simulation methods like atom-continuum or mesoscale-continuum and connecting knowledge from simulations to experiments. Current materials science research questions are related to plasticity of crystalline materials. In the past and present this has included mechanical aspects of tribological contacts, strain hardening and dislocation multiplication, dislocation grain boundary interaction, development of interatomic potentials to assess energetics and dynamics of crystalline defects on the atomic level, and data fusion from simulation and experiment to understand and quantify observed material behavior from simulations and experiments. Research questions on the methodical side revolve around appropriate data formats, standardization and representation of information.

▸ Competences

- Plasticity modeling with mesoscale simulations and scale bridging
- Validation of interatomic potentials based on machine-learning methods
- Simulation of atomistic processes
- Data fusion from simulations and experiments

In order to connect the existing research capabilities of the group with existing initiatives at Ruhr-University, the first grant application in 2020 was a supplementary project within the Collaborative Research Centre SFB/TR-103 "From atoms to turbine blades – a scientific basis for a new generation of single-crystal superalloys" called *Micromechanical Analysis of dislocation networks on dynamic γ/γ´ interfaces*. Methodically, the proposed project couples discrete dislocation dynamics with a simplified creep model for plasticity with phase field simulations for interface motion. This coupling of methods enables the dynamical assessment of dislocation networks which develop around particles, including the driving forces for experimentally observed grooves and ledges at interfaces.

Ongoing projects with national and international collaborators are the application of a neural network potential for pure magnesium to analyze prismatic slip and other dislocation phenomena, thereby probing the application limits and possible issues of this approach. The field of machine-learned interatomic potentials is very dynamic and many methodological and practical

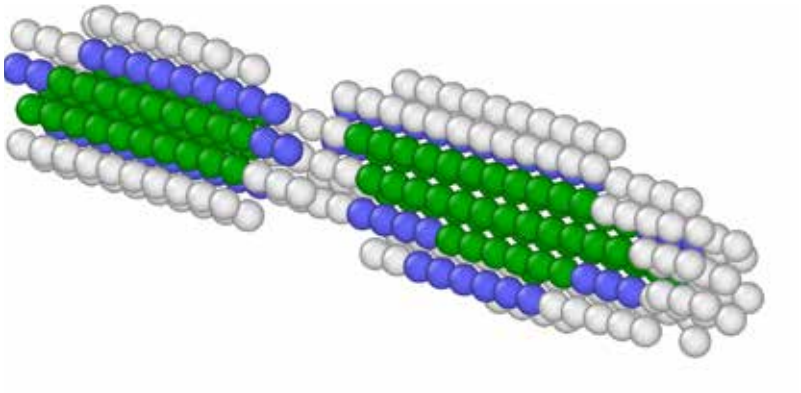


Fig. 9.1: Snapshot from a nudged elastic band (NEB) simulation of the basal cross-slip process in pure Magnesium calculated with a Behler-Parrinello neural network interatomic potential. Colors indicate crystallographic arrangement with green: face-centred cubic; blue: body-centred cubic; grey: others; hexagonally close packed atoms are not shown.

questions are still open. By fitting, validating, and using a neural network-based interatomic potential for pure Mg in the formulation of Behler-Parrinello we could show that a curated training data set based on metallurgical considerations and rigorously following the fitting procedure can produce a very good interatomic potential with close to quantum mechanical accuracy for energies and forces. The potential was subsequently applied to the challenging problem of prismatic cross-slip in Mg and experimental observations about the process could be confirmed and extended.

The group is also involved in the continued development of librascal, a library for the calculation of atomic structure representations for machine learning in the context of atomistic simulations. Many different codes are available for the calculation of atomic scale descriptors as used in machine learning approaches. A meaningful comparison is therefore currently not possible since accuracy and speed of an individual approach is not only a measure of its quality to describe atomic environments but is mixed with issues of implementation in code. Librascal intends to solve this issue by providing a modular framework and readily usable functionality like neighbor lists. It is therefore an ideal basis for implementing new ideas and for meaningful comparison of different descriptor formulations. The first public performance assessment is the comparison of librascal to an existing implementation of the SOAP-GAP (smooth overlap of atomic position – Gaussian approximation potential) approach to predict energies and forces of atomic systems.

Planned projects in the near future are related to atomic descriptors, especially their application to defect analysis in multi-component alloys, the assessment of suitable descriptors and suitable data formats for the description of microstructures from simulations and experiments.

ICAMS

Advanced Study Group Ab Initio-Based Modelling

10. Advanced Study Group Ab Initio-Based Modelling

Prof. Dr. Jörg Neugebauer
Dr. Tilmann Hickel

▸ Research

The Advanced Study Group (ASG) Ab Initio-Based 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 atomic-based mechanisms that determine the microstructure in structural and functional materials 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 chemical, magnetic and structural degrees of freedom for the phase equilibrium in hard-magnetic materials (*Fig. 10.1*). At the same time, the chemical complexity and atomic structure of confined and extended defects in various metals are addressed with novel approaches (*Fig. 10.2*). Hardening mechanisms such as the mechano-chemical coupling during precipitate formation, as well as degradation mechanisms such as hydrogen embrittlement were jointly investigated.

Since the underlying highly accurate and computationally efficient methods require complex simulation protocols, the ASG has developed over the last years pyiron – a platform that provides an integrated development environment to implement, test and employ computational tools such as empirical potentials of multicomponent alloys (*Fig. 10.3*). It does not only provide the user with a standardized 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, in particular with ICAMS, is supported. Consequently, these concepts form a core component of large-scale initiatives like Plattform MaterialDigital and the National Research Data Infrastructure for Materials Science & Engineering (NFDI-MatWerk).

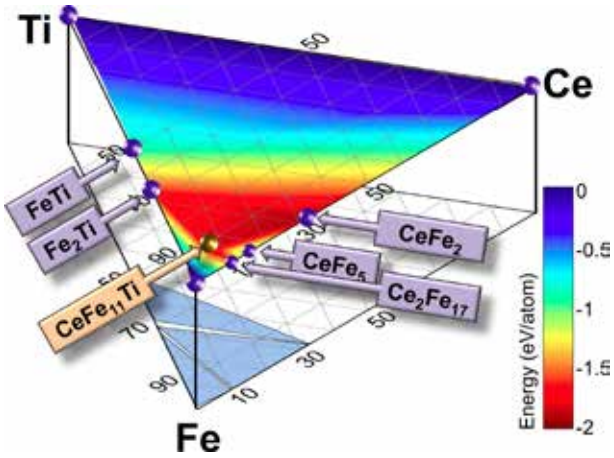


Fig. 10.1: Within the ASG advanced ab initio-based thermodynamic methods are used to predict the phase stability in multi-component alloys. Here, the competition of the hard magnetic phase CeFe11Ti and various binary (e.g. Laves) phases in the Ce-Fe-Ti system at 1500 K is displayed. Blue (red) color shows the energetically high (low) phases among the considered alloys.

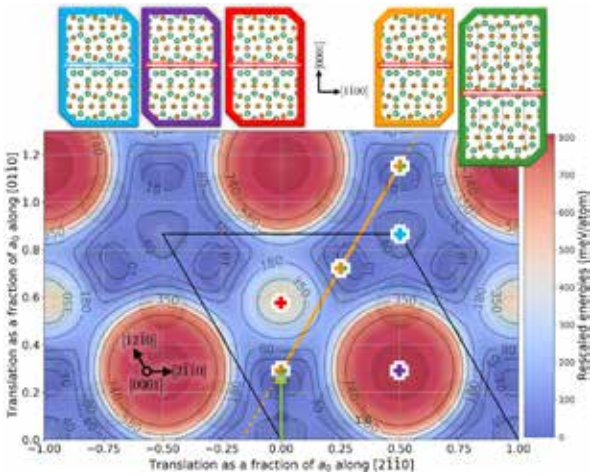


Fig. 10.2: DFT calculation of the basal gamma surface for the planar defects in Nb-rich NbFe2 (35 at.% Nb). The orange-green crosses indicate structures that reproduce the experimentally observed structural features in at least one orientation.

Fig. 10.3: By using the integrated development environment pyiron, the modelling strategies become easily readable in interactive notebooks (middle). They provide a direct link to the physical concepts and raw data (left) as well as to the final results appearing in publications (right).

ICAMS

Advanced Study Group Input Data and Validation

11. Advanced Study Group Input Data and Validation

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

The Advanced Study Group (ASG) "Input Data and Validation" performs research on processing, microstructures and properties of structural and functional engineering materials. In the center of our interest is the formation and evolution of materials' microstructures. We interact with other ICAMS groups and provide experimental data for joint research activities. Although the Covid-19 pandemic hampered scientific face–to–face interaction as well as the conduction of experiments where several scientists work together at close distance, good scientific progress was maintained throughout the reporting period.

In this report, we present research examples from three different fields. In the first one, we consider chemically complex shape memory alloys (SMAs). Generally, shape-memory research presents one of the main scientific areas where members of the Advanced Study Group "Input Data and Validation" have maintained good international visibility for several decades. Within the last years, the concept of high entropy alloys (HEAs) has been adapted successfully to SMAs, derived from binary Nickel-Titanium. SMAs represent a class of functional materials that can re-establish a pre-programmed geometry after a large (apparently plastic) deformation. HEAs refer to a relatively young class of materials. In contrast to conventional alloys, they do not consist of one base-element to which small amounts of other elements are added. Instead, they typically contain equimolar amounts of five or six different elements. HEAs show promising mechanical properties. Recently, we have been able to develop a new high entropy SMA that contains six different elements. This material exhibits shape memory strains which significantly exceed those of binary NiTi SMAs. Our research on chemically complex SMAs is conducted within the DFG priority program SPP 2006 "Compositionally Complex Alloys – High Entropy Alloys (CCA-HEA)". *Figure 11.1* shows our group members preparing materials for research on phase formation and interdiffusion in high entropy SMAs.

Fig. 11.1: Arc melting. Hannah Mittag and former MSS student Oluwaseyi Oluwabi preparing alloys for research on chemically complex shape memory alloys.

As a second research example, we consider Nickel-based superalloys. Superalloys represent key materials for modern gas turbines. 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 center SFB/Transregio 103 (Superalloy Single Crystals – From Atoms to Turbine Blades), which is in its third funding phase. In the present phase, the application of data science approaches for the analysis and interpretation of microstructures and thermo-mechanical properties represents one of the new research directions. For example, we apply machine learning procedures to analyze the growth behavior of dendrites. In a first step, optical micrographs of as-cast superalloys are obtained by a tomographic metallographic procedure. In a second step, neuronal network-based techniques are used to detect and to evaluate the growth behavior of a large number of individual dendrites. This approach not only allows to trace the evolution of microstructures. Moreover, one can detect rare events like spontaneous dendrite deformation processes. *Figure 11.2* shows an example of how tomographic analysis is applied to evaluate the growth behavior of dendrites.

Third example: shape memory polymers are a fascinating class of functional materials, which exhibit similar properties as SMAs; however, they represent polymers. Within the ICAMS/Bochum-based framework of the priority program SPP 1713 ("Strong coupling of thermo-chemical and thermo-mechanical states in applied materials"), members from the ASG "Input Data and Validation" and the group of Fathollah Varnik study how small molecules interact with functional groups within the molecular structure. Members of our ASG have developed an experimental setup that allows investigating the shape memory performance of the polymer actuator, where the material is exposed to low concentrations of various molecular substances in presence/absences of external loads. The group of Fathollah Varnik uses molecular dynamics simulations to analyze the relevant processes on an atomic scale. This joint approach aims for a better understanding of actuation mechanisms, and it will be used to promote shape memory polymers for new engineering applications.

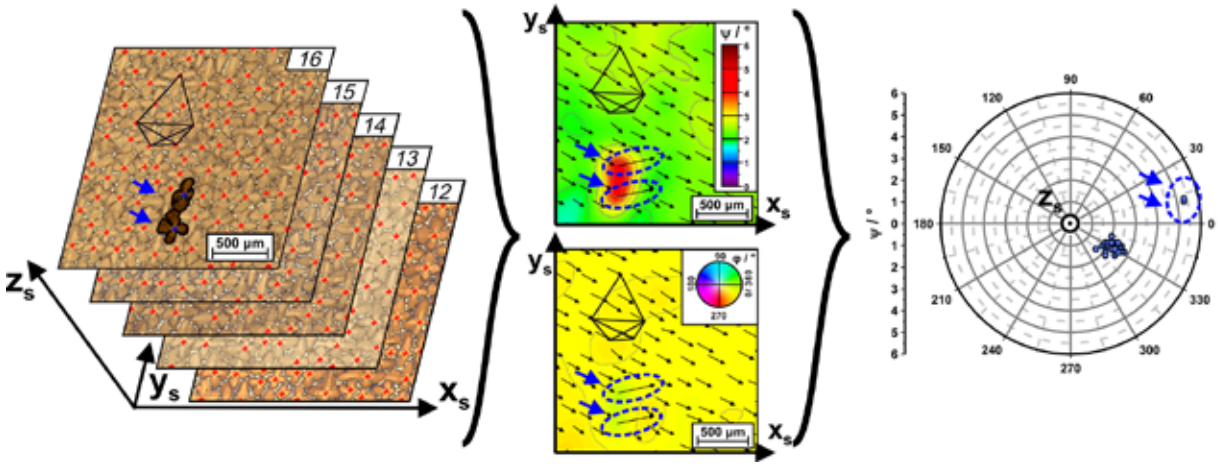


Fig. 11.2: Evaluation of tomographic microstructural information (PhD thesis of Felicitas Scholz). The growth directions of dendrites (marked by small red crosses in optical micrographs) are analyzed in terms of polar and azimuth angles. Two isolated dendrites marked by blue arrows are characterized by growth trajectories which slightly deviate from the main solidification direction.

Fig. 11.3: Scientists from ASG "Input Data and Validation" and from the STKS group "Theory and Simulation of Complex Fluids" involved in shape memory polymer research: Klaus Neuking, Gunther Eggeler, Fathollah Varnik, Axel Marquardt, Elias Mahmoudinezhad, Yucen Shen and Hakan Dumlu.

IC∧MS

Advanced Study Group Processing and Characterisation

12. Advanced Study Group Processing and Characterisation

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

▸ Research

The research activities of the ASG Processing and Characterisation, located at the Steel Institute (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 alloy 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.

By 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 finite element 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 developments and applications of the Integrative Computational Materials Engineering (ICME). The ultimate research focus of these projects lies on establishing an accurate and efficient computational modelling platform for designing and optimising the manufacturing processes necessary to produce tailored material microstructures that provide customized mechanical properties through identifying the correlations between process parameters, material microstructures and mechanical properties. Microstructure-sensitive fatigue simulations have been conducted by using the combination of RVEs and crystal plasticity (CP) finite element simulations to quantitatively evaluate the microstructural effects (phase fraction, grain size, grain shape, inclusion morphology, etc) on fatigue properties of different steels. As a recent application example, the modelling approaches have been further developed to quantify the effects of residual stresses between inclusions and the steel matrix developed during steel production processes on the fatigue properties of a bearing steel, as shown in (*Fig. 12.1*).

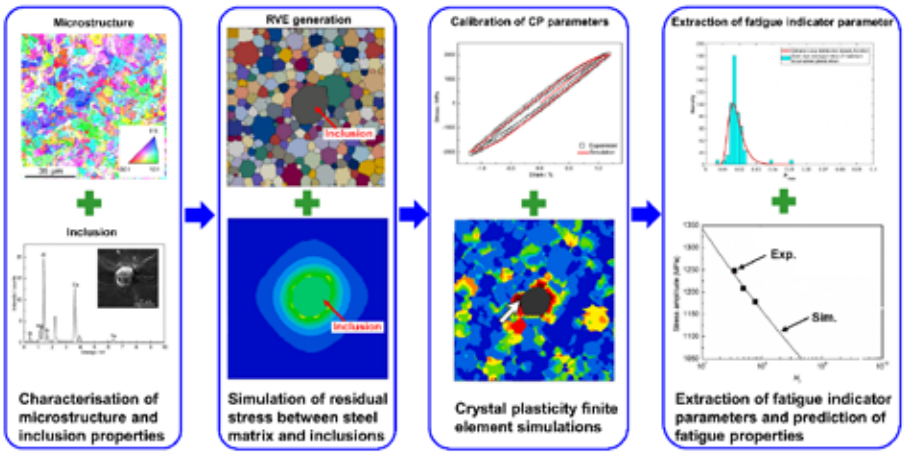


Fig. 12.1: Schematic illustration of the flow chart in microstructure-sensitive fatigue simulations considering the influence of inclusions and residual stresses.

In addition to the material behaviour during conventional processing, the ICME approach has also been established for additive manufacturing (AM) and related applications by the ASG. As schematically shown in (*Fig. 12.2*), we developed a methodology that allows for determination and prediction of process-(micro)structure-properties-performance (PSPP) linkages of AM metals. Numerous computational methods are applied and integrated to consider the AM-specific processing conditions and related microstructural features. These include evaluation of alloy design (CALPHAD method), processing fields during AM (finite element method, computational fluid dynamics), microstructure evolution (phase field, cellular automaton, kinetic Monte Carlo), mechanical behaviour (crystal-plasticity modelling), and structure performance (finite element method) depending on the thermo-chemical-mechanical (TCM) service load. Based on the comprehensive ICME loop and in connection with experimental studies, data-driven models are applied to explore the vast space of potential design parameter combinations. The ASG's AM activities are carried out within the interdisciplinary Research Center for Digital Photonic Production (RCDPP) at RWTH Aachen University. Ongoing research projects focus on the development of steels, Cu, Ni, high-entropy alloys, and light metals for AM; amongst others within national and international collaborative research projects coordinated by the ASG, e.g. EU-H2020 project 'topAM - Tailoring ODS materials processing routes for additive manufacturing of high temperature devices for aggressive environments' and the BMBF-funded NanoMatFutur research group 'MatAM – Design of additively manufactured high-performance materials for the automotive industry'.

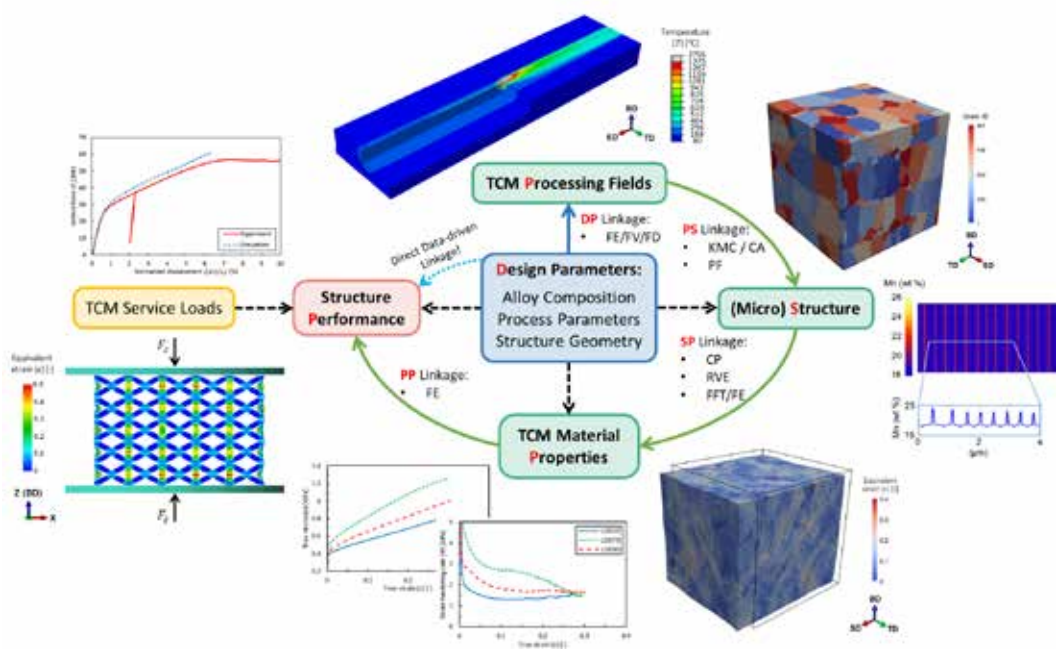


Fig. 12.2: Schematic illustration of the ICME-based approach to determine and predict the PSPP linkage in additively manufactured alloys. The example shows an austenitic steel lattice structure manufactured by laser powder bed fusion.

In order to extend the concept of the ICME to the service life, ICME is combined with the concept of the Integrated Structural Health Engineering (ISHE). Both concepts are evolved in parallel within the Cluster of Excellence - Internet of Production (IoP) - with the aim of an interlink between manufacturing and usage properties. In order to predict the structural health of a component, a defect-based modelling approach (defect engineering) has to be applied in addition to the ICME-based microstructure models. Therefore, we integrate usage data, geometry and relevant defects of a material into the Digital Material Twin. The complex interlinks between the different life phases of the material and the huge amount of collected data make it necessary to reduce the data to a lower complexity in order to be able to process it in real time. The condensed knowledge, gained from the digital material twin, is called digital material shadow, which represents only the part of the data that is relevant to the current problem. The digital material shadow helps us to connect characterization and simulation in real time. The newly formed interlinks result in a higher level of understanding of cross-domain relationships due to real-time availability from various process steps. At IEHK, a new database is set up to store semantically adequate data, from our test facilities, which is integrated and automated, to achieve a user-independent online characterization, and accelerate the material development.

ICAMS

Advanced Study Group Diffusion and Microstructure Analysis

13. Advanced Study Group Diffusion and Microstructure Analysis

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

▸ Research

The Advanced Study Group Diffusion and Microstructure Analysis is located at the Institute of Materials Physics of the Westfälische Wilhelms-Universität Münster. It employs a range of complementing experimental methods to analyze the underlying physical mechanisms and microstructural origins of macroscopic materials behavior.

Specific emphasis is on the coupled analysis of
- atomic transport,
- atomic-level structure
- 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 2020 the studies were focused on three main topics described below.

Impact of room temperature high-pressure torsion on the relaxation of glassy and supercooled liquid states of PdNiP

Relaxation of different states in a $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass deformed by room temperature high-pressure torsion was investigated in detail by means of XRD, DSC, low-temperature heat capacity measurements and TEM using fluctuation electron microscopy. Unique medium range order (MRO) characteristics of the individual glassy states were revealed, (*Fig. 13.1*). The calorimetric signals are traced back to the modifications of the short-range order including the MRO on an unprecedentedly detailed level that allowed analysis of the glass response in terms of potential energy landscape (*Fig. 13.2*).

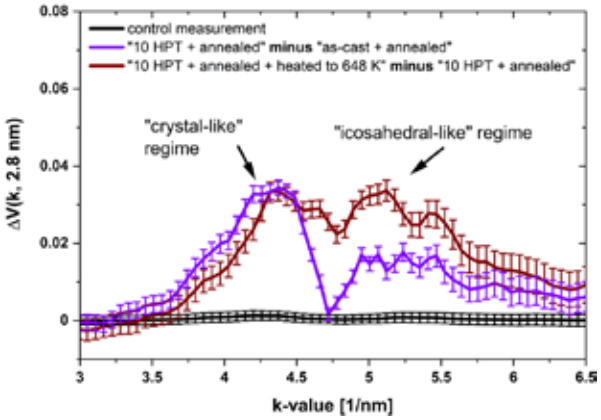


Fig. 13.1: Normalized variance difference curves, ΔV (k) using exemplarily the probe size of 2.8 nm in order to show the reproducibility by two different data sets of the as-cast state as well as the significant changes for differently treated samples in terms of icosahedral and crystal-like dominated MRO at this probe size.

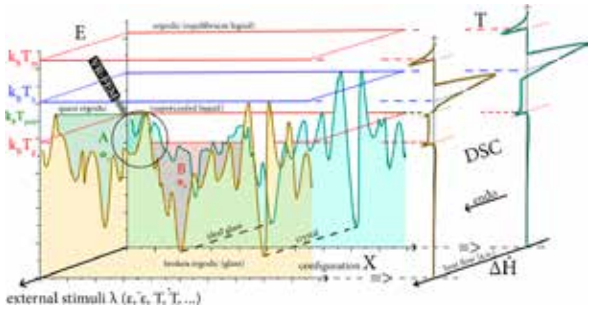


Fig. 13.2: A schematic 3D illustration of the PEL showing the dependence of the total potential energy E as function of the configurational parameter X and an external action λ corresponding to the underlying thermo-mechanical history. The VR-FEM provides a unique tool to inspect atomistic structures within the PEL, especially their evolution.

Grain boundary diffusion and grain boundary structures of a Ni-Cr-Fe-alloy: Evidences for grain boundary phase transitions

The grain boundary structure-property relationship was studied in a Ni-base 602CA coarse-grained alloy using a novel correlative tracer diffusion-analytical microscopy approach. Co-existence of several short-circuit contributions to tracer diffusion was distinguished at higher temperatures. These contributions were related to different families of high-angle grain boundaries with distinct coverages by precipitates and segregation levels as revealed by HAADF-STEM combined with EDX measurements and a detailed atom probe tomography analysis. The work provides solid evidence towards the existence of grain boundary phase transitions (including a spinodal-like GB decomposition with alternating Ni- and Cr-enriched layers, see *Fig. 13.3*) in the Ni-base multi-component alloy.

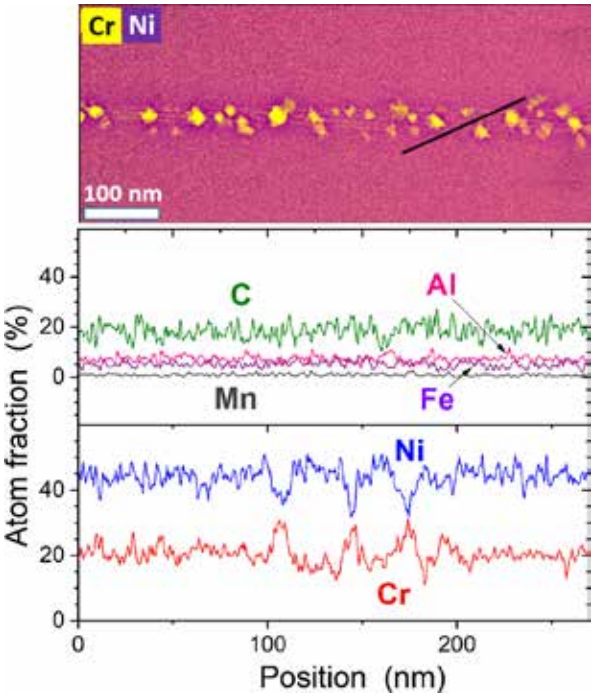


Fig. 13.3: Overlapped Cr and Ni elemental EDS maps of a straight GB after annealing at 873 K for 18 h of a Ni-Cr-Fe-based alloy (upper panel). A line-scan was performed along the black line and the measured atomic fractions are plotted (bottom panel). The grain boundary is inclined with respect to the beam that allowed resolving the chemical variations in the boundary plane. their evolution.

Grain boundary diffusion in CoCrFeMnNi high entropy alloy: kinetic hints towards a phase decomposition

Grain boundary diffusion of all principal elements in a coarse-grained equiatomic CoCrFeMnNi high entropy alloy is measured in a wide temperature range. The results prove that the absence of element segregation at higher temperatures and verify that the grain boundary width is about 0.5 nm. Two distinct contributions were observed at lower temperatures that hint towards a phase decomposition at a fraction of high-angle grain boundaries at these conditions. The results are discussed in terms of the existence of a structural multiplicity of high-angle grain boundaries.

A correlative microscopy combining transmission Kikuchi diffraction and APT manifests formation of neighbouring Ni-Mn-rich and Cr-rich precipitates at high-angle grain boundaries (*Fig. 13.4*).

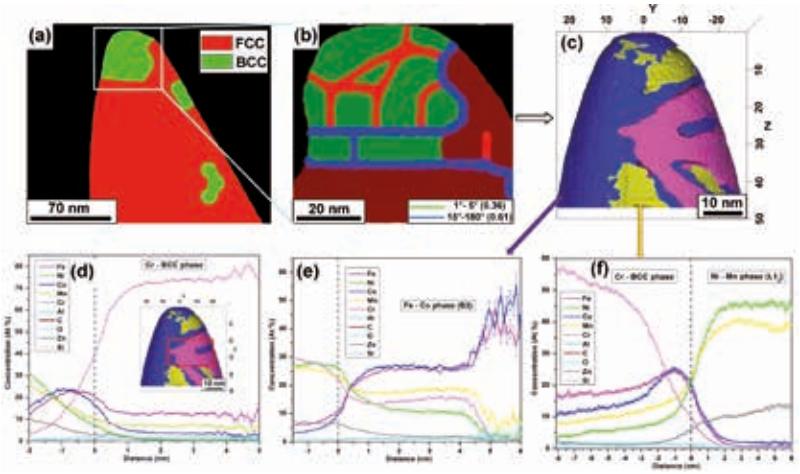


Fig. 13.4: (a) TKD phase map of the two-phase region enlarged in (b) with image quality (IQ) overlap on the phase map revealing the GBs (c) the corresponding 3D reconstruction of constituent elements obtained from APT with individual enrichments highlighted using Cr 42 at%, Co 11 at% and Mn 24 at.% isoconcentration surfaces (d) proximity histogram obtained from the Cr-enriched bcc phase (the rectangle shows the Cr rich region in the inset). (e) proximity histogram of the Fe-Co-rich region indicated by an angled arrow from (c) and (f) proximity histogram of the Mn-enriched region indicated by the straight arrow.

ICAMS

Advanced Study Group Continuum Mechanics

14. Advanced Study Group Continuum Mechanics

Prof. Dr.-Ing. Daniel Balzani
Prof. Dr. Klaus Hackl
Dr.-Ing. Philipp Junker

▸ Research

In 2020, the advanced study group „continuum mechanics“ started working, and since then, several meetings have taken place to initiate collaborations. Currently, joint research between Fathollah Varnik and Haifeng Wang from ICAMS and the group of Daniel Balzani (Chair of Continuum Mechanics, RUB) computationally analyzes material degradation in diseased arteries, in particular aneurysms. It is well known that arteries suffer from microscopic damage when loading exceeds the physiological range. This microscopic damage results in a weakening of the tissue, rendering the artery more flexible under similar loading. Due to the weakened arterial wall of an aneurysm and high blood pressure, as usually observed in patients with aneurysms, a supra-physiological loading scenario can be expected in aneurysms. Therefore, microscopic damage effects may be hypothesized in such cases, which in turn may lead to further weakening of the tissue. The computational analysis of the complex mechanical phenomena in an aneurysm in an initial phase in connection with the blood flow is thus the goal of this collaboration, in order to study to what extent tissue degradation may contribute to the progress of aneurysms. To this end, a material model for the description of the microscopic damage at the material point [Balzani et al. Comput. Methods Appl. Mech. Engrg. 2012] was implemented in the software package SimVascular (www.simvascular.org). Based on the implementation, first simulations were performed on simplified benchmark arteries considering damage in the tissue, and, currently more complex geometries are studied (*Fig. 14.1*).

Apart from this research, further collaboration is expected in the context of simulating phase transformations. Here, different conceptual approaches from the group of Ingo Steinbach (ICAMS) and Klaus Hackl (Chair of Material Theory) are considered to be compared with a view to accuracy and efficiency. A recent successful example of this collaboration is the large deformation framework applied to martensitic transformation [Shchyglo et al. Acta Mater. 2019]. These results will be compared to effective energies of martensitic microstructures calculated in [Govindjee et al. Continuum Mech. Thermodyn. 2007].

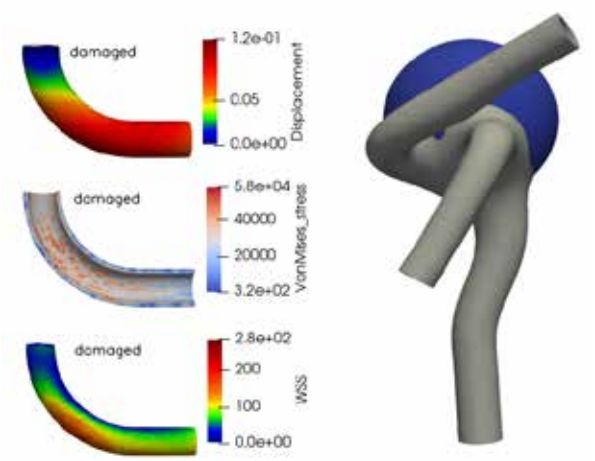


Fig. 14.1: Exemplary simulation results of a simplified artery with blood flow and degenerating tissue (left) and a more complex artery with an aneurysm (right).

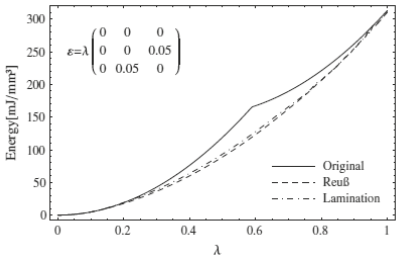
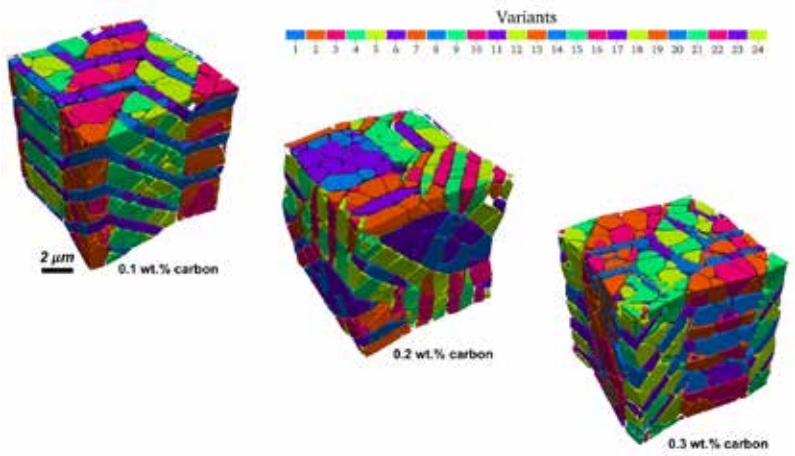


Fig. 14.3: Relaxed and unrelaxed energies; relaxed energies computed by lamination upper and Reuß lower bound [Govindjee et al. Continuum Mech. Thermodyn. 2007].

Fig. 14.2: Phase-field Simulation for martensite microstructures of steel for different carbon content. [Shchyglo et al. Acta Mater. 2019].



ICAMS

Research Highlights

15. Research Highlights

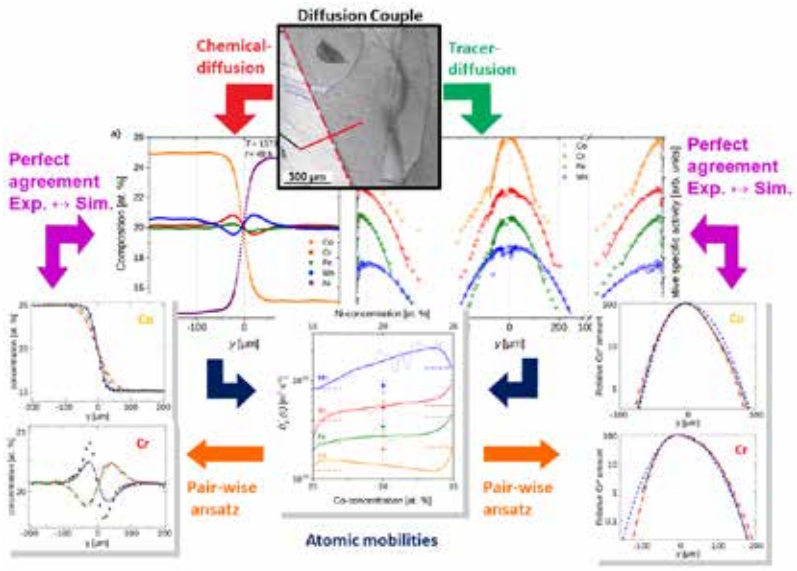
2019

Concentration-dependent atomic mobilities in FCC CoCrFeMnNi high-entropy alloys

D. Gaertner, K. Abrahams, J. Kottke, V. A. Esin, I. Steinbach, G. Wilde, S. V. Divinski

Acta Materialia, **166**, 357-370 (2019)

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. As a result, the composition-dependent tracer diffusion coefficients of Co, Cr, Fe and Mn are determined. The elements are characterized by significantly different diffusion rates, with Mn being the fastest element and Co being the slowest one. The elements having originally equiatomic concentration through the diffusion couple are found to reveal up-hill diffusion, especially Cr and Mn. The atomic mobility of Co seems to follow a S-shaped concentration dependence along the diffusion path. The experimentally measured kinetic data are checked against the existing CALPHAD-type databases. In order to ensure a consistent treatment of tracer and chemical diffusion a generalized symmetrized 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.

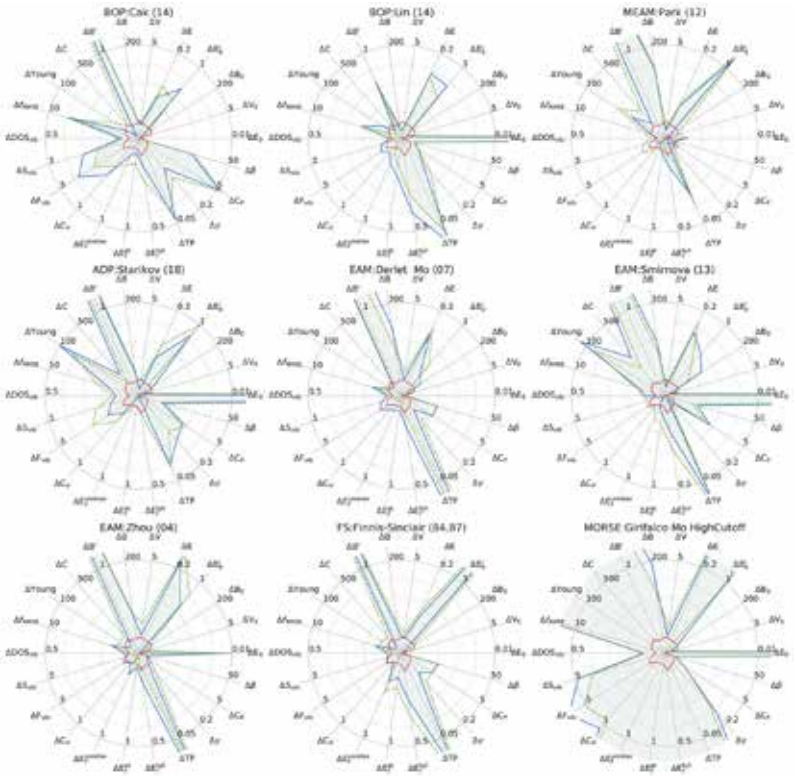


Combined radiotracer- and interdiffusion measurement and simulation in CoCrFeMnNi high-entropy alloy.

Transferability of interatomic potentials for molybdenum and silicon

Y. Lysogorskiy, T. Hammerschmidt, J. Janssen, J. Neugebauer, R. Drautz
Modelling and Simulation in Materials Science and Engineering, **27**, 25007 (2019)

Interatomic potentials are widely used in computational materials science, in particular for simulations that are too computationally expensive for density functional theory (DFT). Most interatomic potentials have a limited application range and often there is very limited information available regarding their performance for specific simulations. We carried out high-throughput calculations for molybdenum and silicon with DFT and a number of interatomic potentials. We compare the DFT reference calculations and experimental data to the predictions of the interatomic potentials. We focus on a large number of basic materials properties, including the cohesive energy, atomic volume, elastic coefficients, vibrational properties, thermodynamic properties, surface energies and vacancy formation energies, which enables a detailed discussion of the performance of the different potentials. We further analyze correlations between properties as obtained from DFT calculations and how interatomic potentials reproduce these correlations, and suggest a general measure for quantifying the accuracy and transferability of an interatomic potential. From our analysis we do not establish a clearcut ranking of the potentials as each potential has its strengths and weaknesses. It is therefore essential to assess the properties of a potential carefully before application of the potential in a specific simulation. The data presented here will be useful for selecting a potential for simulations of Mo or Si.



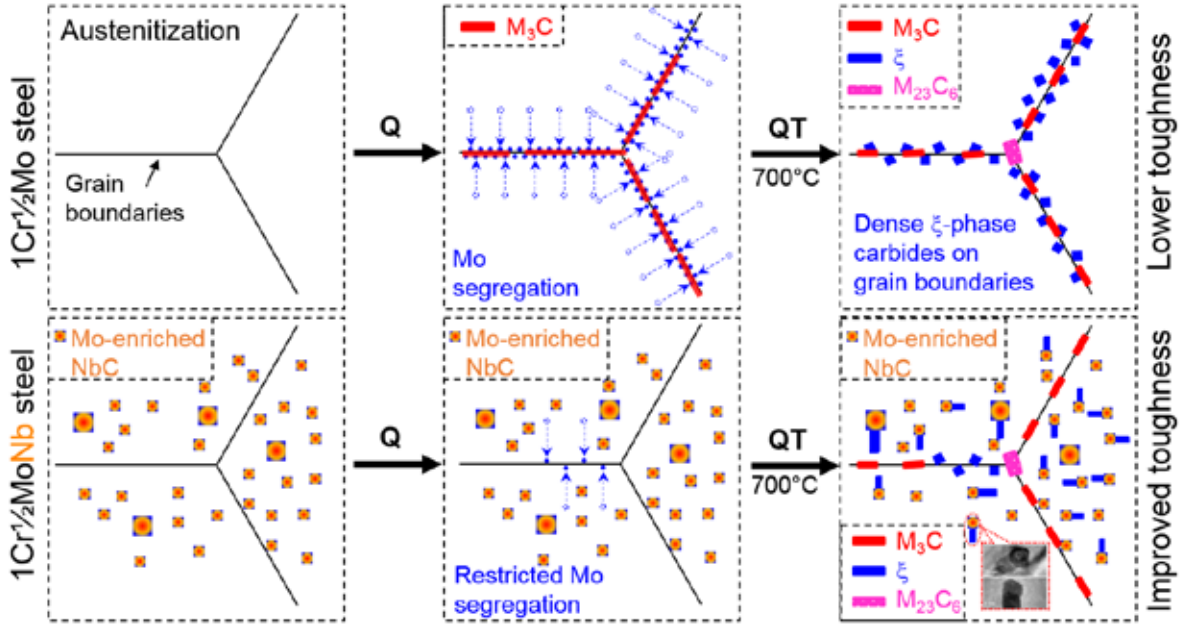
Errors for the considered properties as calculated by interatomic potentials with respect to GGA-PBE (blue solid line) and LDA (orange dashed line).

Effect of Nb on improving the impact toughness of Mo-containing low-alloyed steels

H. C. Wang, C. Somsen, Y. J. Li, S. G. Fries, E. Detemple, G. Eggeler
Journal of Materials Science, **54**, 7307-7321 (2019)

The microalloying of low-alloyed steels with Nb can improve the strength-to-toughness balance. Such an effect of Nb is usually ascribed to the refinement of the grain structure occurring in the austenite regime during hot forming. In the present work, we report that Nb enhances the impact toughness of a low-alloyed Cr–Mo steel by a mechanism which has not been appreciated so far. The lower impact toughness in the Nb-free Cr–Mo steel is due to segregation of Mo to boundaries, which facilitates the formation of fine Mo-rich ξ-phase carbides lining up along the boundaries. This further promotes the nucleation and propagation of microcracks. The addition of Nb leads to the formation of Mo-enriched NbC particles. The interfaces between these particles and the matrix supply new preferential sites for precipitation of Mo-rich ξ-phase carbides upon subsequent tempering. In this way, Nb additions result in a decrease of Mo segregation to boundaries, significantly reducing the precipitation of ξ-phase carbides on grain boundaries, thus leading to improved impact toughness. In addition to the classical microstructural explanation (grain size effect), this chemical role of Nb sheds new light on the design strategies of advanced low-alloyed steels with optimized strength-to-toughness ratios.

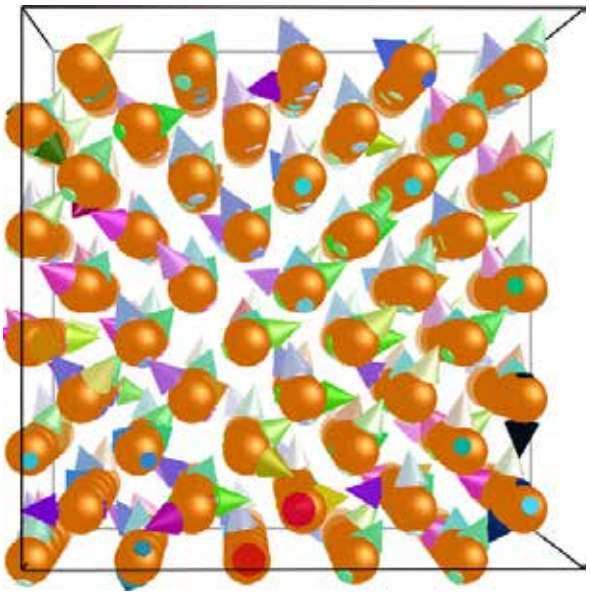
Crystal structure of the C_{14} Laves-phase of Fe_2Nb with Fe atoms in red and Nb atoms in blue. The small spheres indicate possible tetrahedral sites for C and N interstitial atoms.



Accelerating spin-space sampling by auxiliary spin dynamics and temperature-dependent spin-cluster expansion

N. Wang, T. Hammerschmidt, J. Rogal, R. Drautz
Physical Review B,**99**, 94402 (2019)

Atomistic simulations of the thermodynamic properties of magnetic materials rely on an accurate modeling of magnetic interactions and an efficient sampling of the high-dimensional spin space. Recent years have seen significant progress with a clear trend from model systems to material-specific simulations that are usually based on electronic-structure methods. Here we develop a Hamiltonian Monte Carlo framework that makes use of auxiliary spin dynamics and an auxiliary effective model, the temperature-dependent spin-cluster expansion, in order to efficiently sample the spin space. Our method does not require a specific form of the model and is suitable for simulations based on electronic-structure methods. We demonstrate fast warm-up and a reasonably small dynamical critical exponent of our sampler for the classical Heisenberg model. We further present an application of our method to the magnetic phase transition in bcc iron using magnetic bond-order potentials.



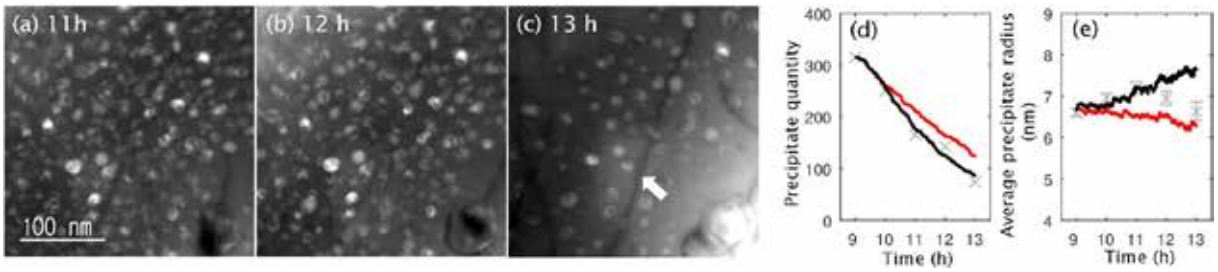
Magnetization of bcc iron at the magnetic phase transition temperature in terms of the spin directions as obtained with a magnetic bond-order potential.

First evidence for mechanism of inverse ripening from in-situ TEM and phase-field study of δ′ precipitation in an Al-Li alloy

J. Park, R. Darvishi Kamachali, S.-D. Kim, S.-H. Kim, C. Oh, C. Schwarze, I. Steinbach

Scientific Reports, **9**, 3981 (2019)

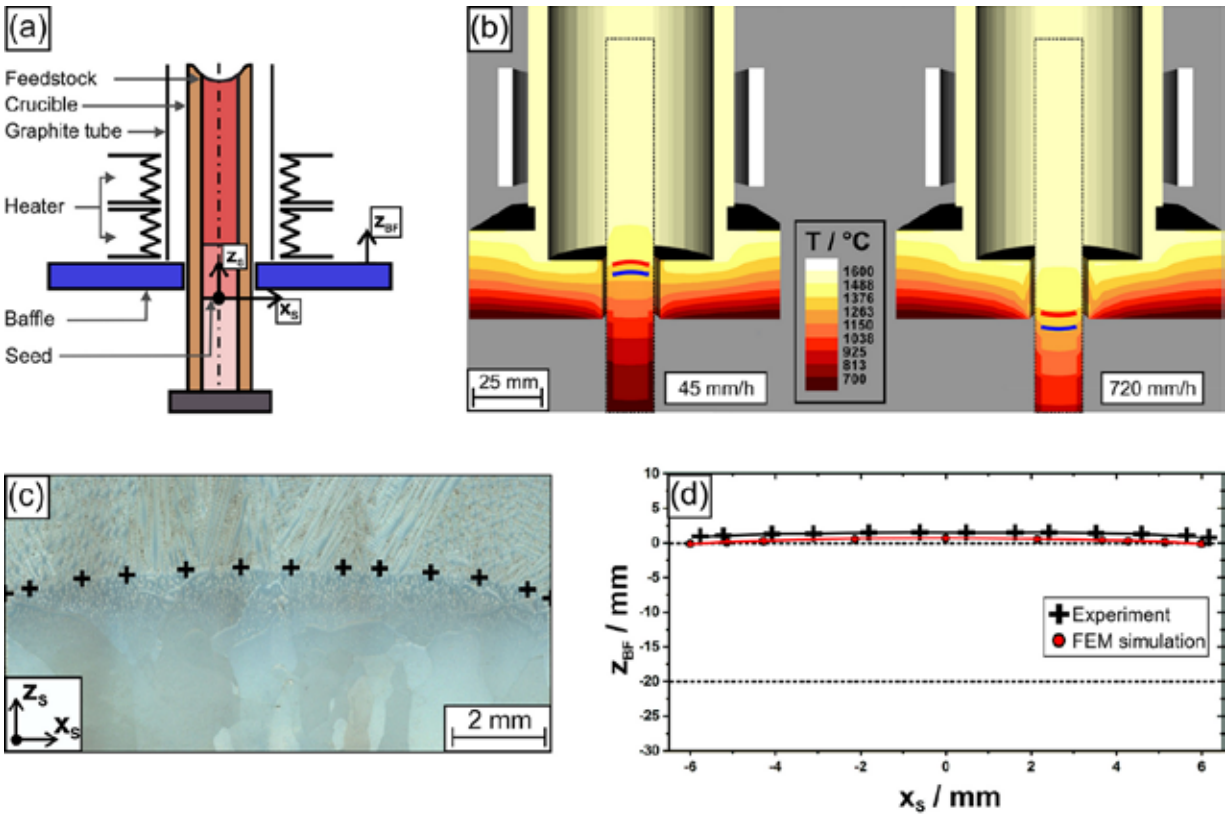
In-situ TEM investigation of aging response in an Al-7.8 at.% Li was performed at 200 °C up to 13 hours. Semi-spherical δ′ precipitates growing up to an average radius of 7.5 nm were observed. The size and number of individual precipitates were recorded over time and compared to large-scale phase-field simulations without and with a chemo-mechanical coupling effect, that is, concentration dependence of the elastic constants of the matrix solid solution phase. This type of coupling was recently reported in theoretical studies leading to an inverse ripening process where smaller precipitates grew at the expense of larger ones. Considering this chemo-mechanical coupling effect, the temporal evolution of number density, average radius, and size distribution of the precipitates observed in the in-situ experiment were explained. The results indicate that the mechanism of inverse ripening can be active in this case. Formation of dislocations and precipitate-free zones are discussed as possible disturbances to the chemo-mechanical coupling effect and consequent inverse ripening process.



Dissolution of the precipitates after (a) 11 hours (b) 12 hours, and (c) 13 hours of aging is shown. The white arrow indicates a dislocation. The number density of the precipitate rapidly decreased between 12 and 13 hours. Evolution of (d) the precipitate quantity (number) and (e) average precipitate radius is presented and compared to the simulation results.

On crystal mosaicity in single crystal Ni-based superalloys

P. Hallensleben, F. Scholz, P. Thome, H. J. Schaar, I. Steinbach, G. Eggeler, J. Frenzel
Crystals, **9**, 149 (2019)



a) Experimental setup of the seeded vertical Bridgman process, b) Numerical results for the temperature field evolution during the Bridgman process with respect to varying withdrawal rates, c) Experimentally determined liquidus isotherm for a withdrawal rate of 45 mm/h, d) Comparison of experimentally determined and simulated liquidus isotherm for a withdrawalrate of 180mm/h.

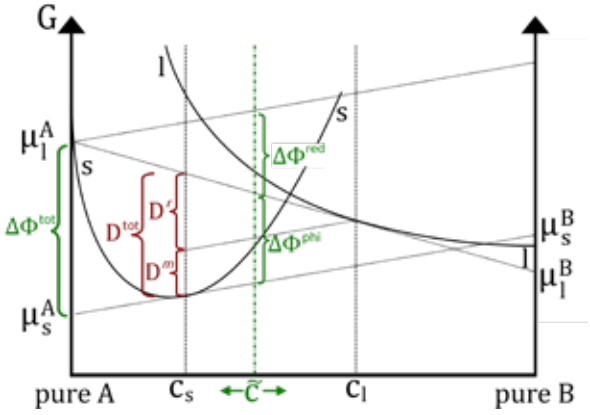
In the present work, we investigate the evolution of mosaicity during seeded Bridgman processing of technical Ni-based single crystal superalloys (SXs). For this purpose, we combine solidification experiments performed at different withdrawal rates between 45 and 720 mm/h with advanced optical microscopy and quantitative image analysis. The results obtained in the present work suggest that crystal mosaicity represents an inherent feature of SXs, which is related to elementary stochastic processes which govern dendritic solidification. In SXs, mosaicity is related to two factors: inherited mosaicity of the seed crystal and dendrite deformation. Individual SXs have unique mosaicity fingerprints. Most crystals differ in this respect, even when they were produced using identical processing conditions. Small differences in the orientation spread of the seed crystals and small stochastic orientation deviations continuously accumulate during dendritic solidification. Direct evidence for dendrite bending in a seeded Bridgman growth process is provided. It was observed that continuous or sudden bending affects the growth directions of dendrites. We provide evidence which shows that some dendrites continuously bend by 1.7° over a solidification distance of 25 mm.

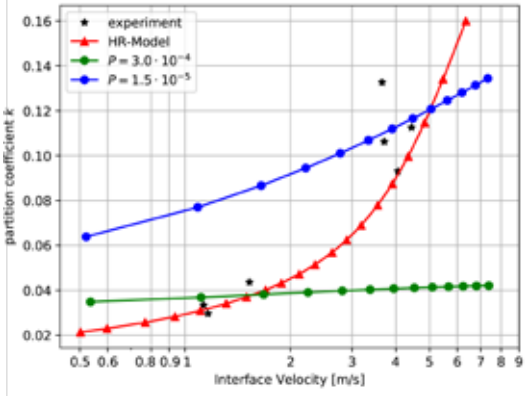
Solute trapping in non-equilibrium solidification: A comparative model study

K. Reuther, S. Hubig, I. Steinbach, M. Rettenmayr
Materialia, **6**, 100256 (2019)

A sharp interface model and a diffuse interface model describing rapid solidification are compared. Both models are based on the assumption of two independent processes at the solid/liquid interface that together consume the available driving force. These two processes are (1) the interface motion and (2) the redistribution of atoms between the two phases. The sharp interface model is based on an interface thermodynamics model (Hillert and Rettenmayr) and derives its driving force for the phase transformation directly from Gibbs free energy formulations of the liquid and solid phases. In contrast, the Finite Interface Disspiation model (Steinbach et al.), a diffuse interface model, is based on a grand potential formulation. The models are benchmarked against experimental data on solute trapping in the Al–Sn system (Smith and Aziz). The sharp interface model reproduces the experimental data with a single set of kinetic parameters, the diffuse interface model requires a velocity dependent interface permeability. It is concluded that due to the investigated high Péclet number regime the permeability in the diffuse interface model does not only describe the transport processes through the interface, but also the diffusion processes in the layer directly in front of it.

Left: Comparison between the thermodynamic driving forces of the investigated sharp and diffuse interface models. In a solidification setting, like it is shown here, the phase field driving forces (green) will be higher than the sharp interface driving forces (red). Right: k-v-curves predicted by phase field and sharp interface model in a rapid solidification setting of an Al-0.2 at.% Sn alloy.



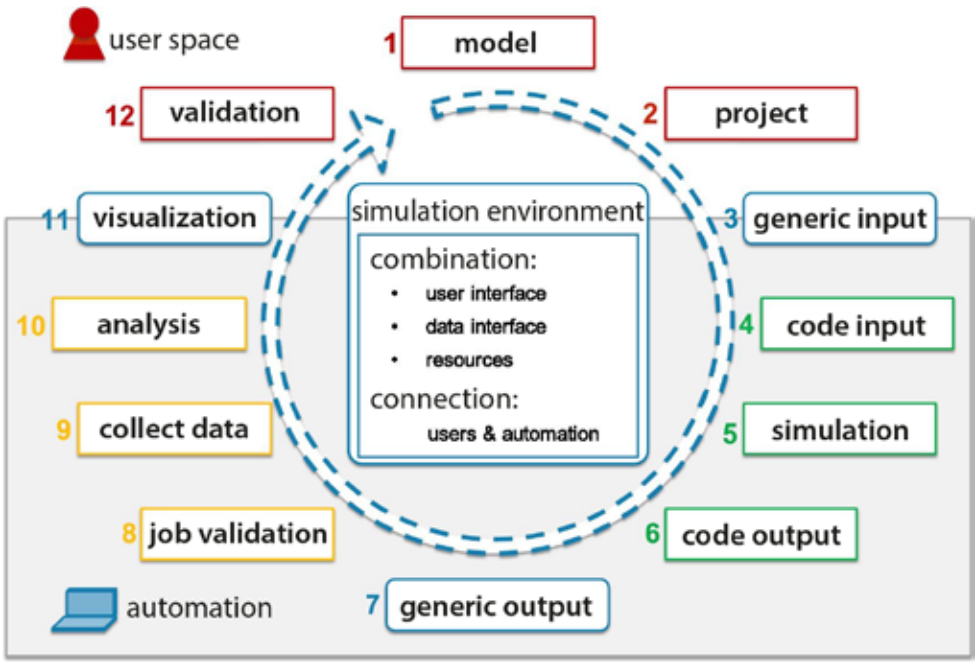


Pyiron: An integrated development environment for computational materials science

J. Janssen, S. Surendralal, Y. Lysogorskiy, M. Todorova, T. Hickel, R. Drautz, J. Neugebauer
Computational Materials Science, **163**, 24-36 (2019)

To support and accelerate the development of simulation protocols in atomistic modelling, we introduce an integrated development environment (IDE) for computational materials science called pyiron (http://pyiron.org). The pyiron IDE combines a web based source code editor, a job management system for build automation, and a hierarchical data management solution. The core components of the pyiron IDE are pyiron objects based on an abstract class, which links application structures such as atomistic structures, projects, jobs, simulation protocols and computing resources with persistent storage and an interactive user environment. The simulation protocols within the pyiron IDE are constructed using the Python

programming language. To highlight key concepts of this tool as well as to demonstrate its ability to simplify the implementation and testing of simulation protocols we discuss two applications. In these examples we show how pyiron supports the whole life cycle of a typical simulation, seamlessly combines ab initio with empirical potential calculations, and how complex feedback loops can be implemented. While originally developed with focus on ab initio thermodynamics simulations, the concepts and implementation of pyiron are general thus allowing to employ it for a wide range of simulation topics.



Schematic view of a typical simulation life cycle, which illustrates the user's interaction with the various simulation tasks. It is divided in twelve steps, from the definition of the model -step 1 to its validation -step 12. Three of these steps require obligatory input from the user, the model definition-step 1, the project definition-step 2, and the validation-step 12, while the rest can be automated. In particular the parsing of input and output data-steps 4 & 6 – as well as the collection of data-step 9 – are common tasks to any simulation. Using an intermediate layer with generic input-step 3, generic output-step 7 – and generalized tools for visualization-step 11, provides an abstraction layer that is code independent.

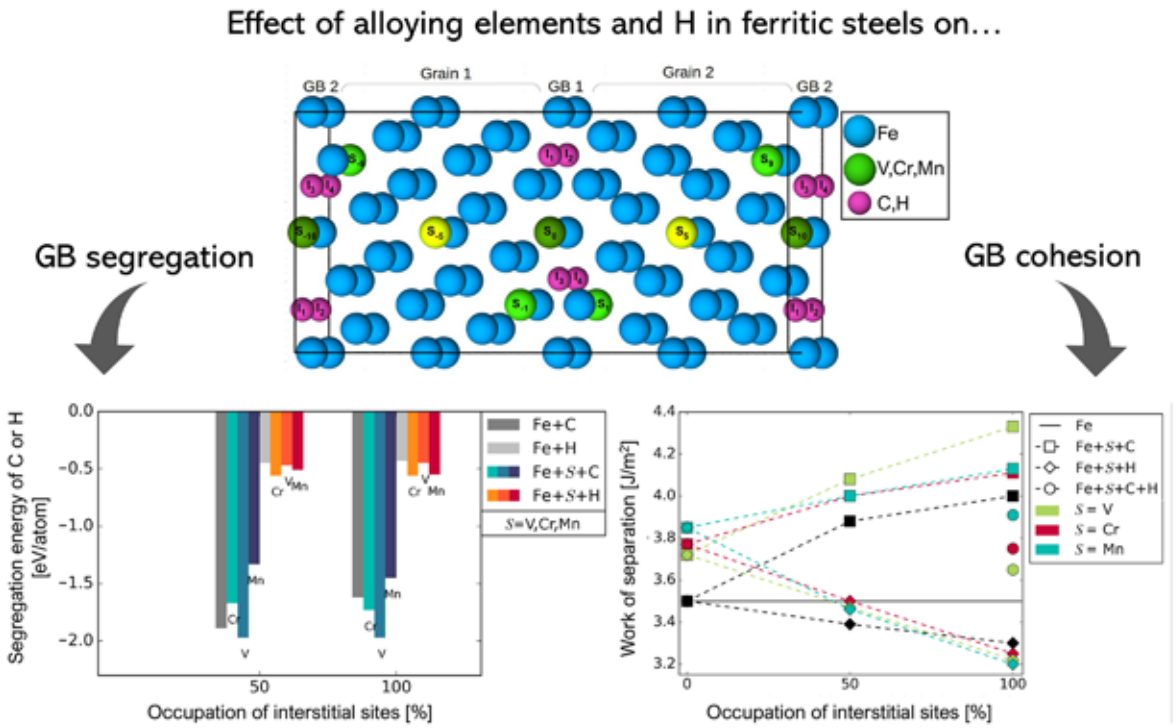
Ab initio study of the combined effects of alloying elements and H on grain boundary cohesion in ferritic steels

A. P. Subramanyam, A. Azócar Guzmán, S. Vincent, A. Hartmaier, R. Janisch

Metals, **9**, 291 (2019)

Abstract: Hydrogen enhanced decohesion is expected to play a major role in ferritic steels, especially at grain boundaries. Here, we address the effects of some common alloying elements C, V, Cr, and Mn on the H segregation behaviour and the decohesion mechanism at a Σ5(310)[001] 36.9 ° grain boundary in bcc Fe using spin polarized density functional theory calculations. We find that V, Cr, and Mn enhance grain boundary cohesion. Furthermore, all elements have an influence on the segregation energies of the interstitial elements as well as on these elements' impact on grain boundary cohesion. V slightly promotes segregation of the cohesion enhancing element C. However, none of the elements increase the cohesion enhancing effect of C and reduce the detrimental effect of H on interfacial cohesion at the same time. At an interface which is co-segregated with C, H, and a substitutional element, C and H show only weak interaction, and the highest work of separation is obtained when the substitute is Mn.

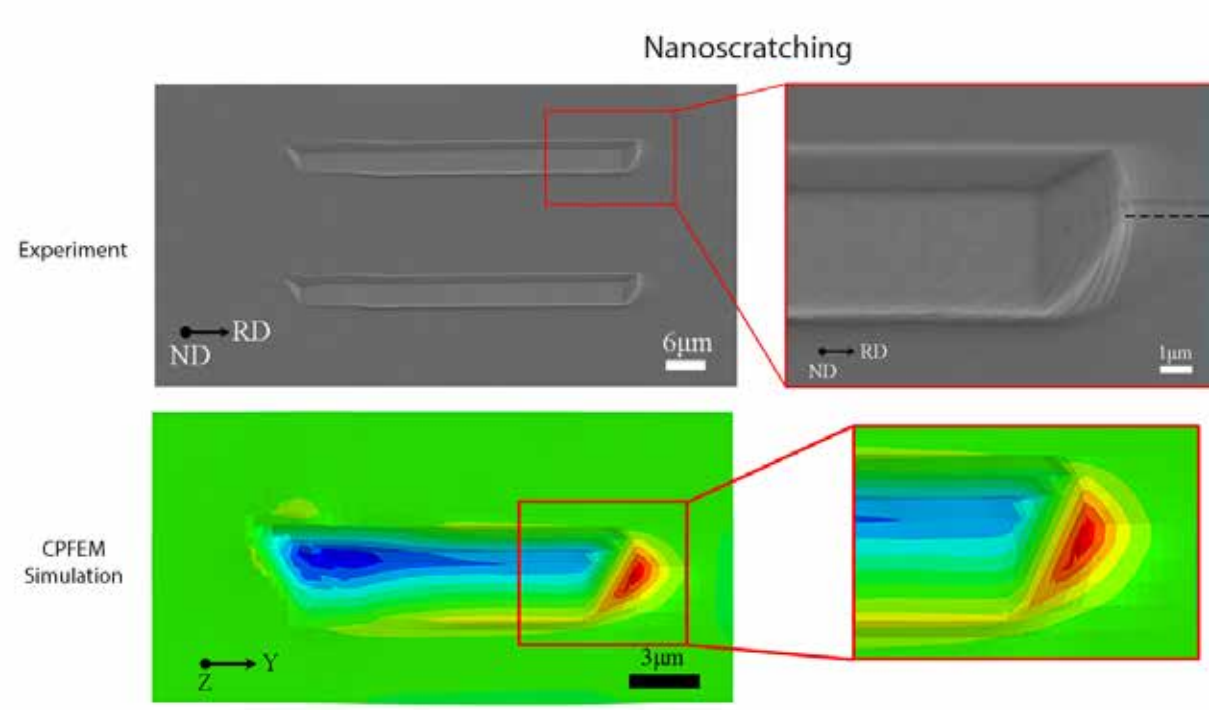
There are two aspects to H segregation at grain boundaries: on the one hand, the interface provides trappings sites for H and thus reduces the freely diffusing H in the microstructure. On the other hand, the trapped hydrogen can reduce grain boundary cohesion. In this study, it was investigated how the alloying elements Cr, V, Mn, and C influence these processes.



Crystal plasticity finite element simulation and experiment investigation of nanoscratching of single crystalline copper

Z. Wang, H. Zhang, Z. Li, G. Li, J. Zhang, J. Zhang, H. u. Hassan, Y. Yan, A. Hartmaier, T. Sun
Wear, **430-431**,100-107 (2019)

Mechanical properties of crystalline materials strongly correlate with deformation behaviour at the grain level. In the present work, we establish a 3D crystal plasticity finite element model of nanoscratching of single crystalline copper using a Berkovich probe, which is capable of addressing the crystallography influence. In particular, nanoindentation experiments and high resolution electron back-scatter diffraction characterization are jointly carried out to precisely calibrate parameters used in the crystal plasticity finite element model. Subsequent finite element simulations of nanoscratching are performed to reveal fundamental deformation behaviour of single crystalline copper in terms of mechanical response and surface pile-up topography, as well as their dependence on crystallographic orientation. Furthermore, nanoscratching experiments with the same parameters used in the finite element simulations are carried out, the results of which are further compared with predication results by the finite element simulations. Simulation data and experimental results jointly demonstrate the strong anisotropic characteristics of single crystalline copper under nanoscratching, due to the crystallographic orientation dependent coupled effects of intrinsic dislocation slip and extrinsic discrete stress distribution by probe geometry.



Qualitative comparison of CPFEM simulation of Berkovich nanoscratching with experimental results.

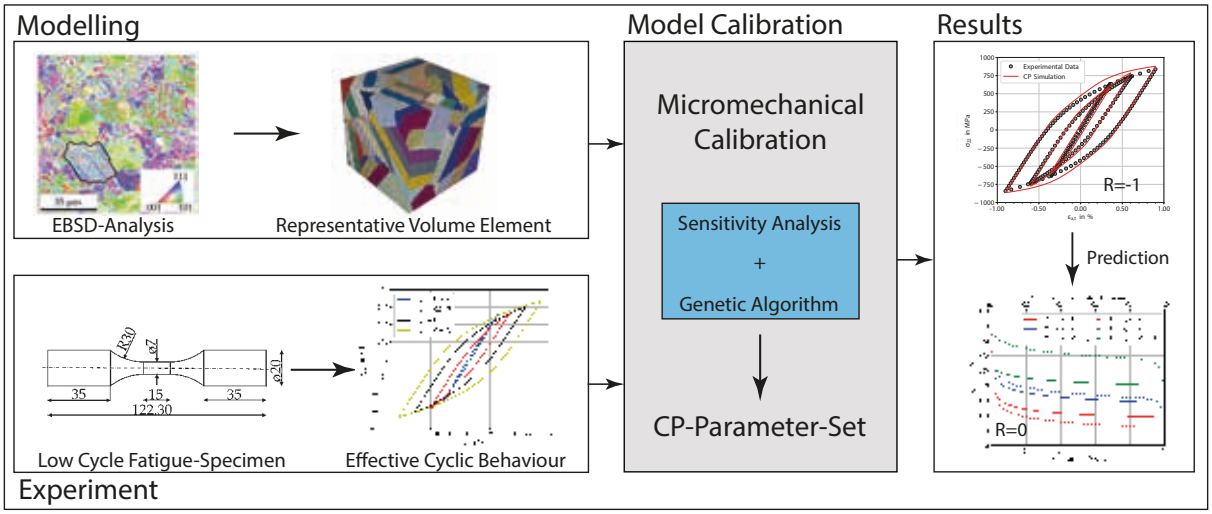
Micromechanical modelling of the cyclic deformation behavior of martensitic SAE 4150 – a comparison of different kinematic hardening models

B. J. Schäfer, X. Song, P. Sonnweber-Ribic, H. u. Hassan, A. Hartmaier

Metals, **9**, 368 (2019)

A fundamental prerequisite for the micromechanical simulation of fatigue is the appropriate modelling of the effective cyclic properties of the considered material. Therefore, kinematic hardening formulations on the slip system level are of crucial importance due to their fundamental relevance in cyclic material modelling. The focus of this study is the comparison of three different kinematic hardening models (Armstrong Frederick, Chaboche, and Ohno-Wang). In this work, investigations are performed on the modelling and prediction of the cyclic stress-strain behavior of the martensitic high-strength steel SAE 4150 for two different total strain ratios (R ε = −1 and R ε = 0). In the first step, a three-dimensional martensitic microstructure model is developed by using multiscale Voronoi tessellations. Based on this martensitic representative volume element, micromechanical simulations are performed by a crystal plasticity finite element model. For the constitutive model calibration, a new multi-objective calibration procedure incorporating a sensitivity analysis as well as an evolutionary algorithm is presented. The numerical results of different kinematic hardening models are compared to experimental data with respect to the appropriate modelling of the Bauschinger effect and the mean stress relaxation behavior at Rε = 0. It is concluded that the Ohno–Wang model is superior to the Armstrong Frederick and Chaboche kinematic hardening model at Rε =−1 as well as at Rε = 0.

Prediction of different mean stress behavior for a martensitic material under cyclic loading using crystal plasticity finite element method and different kinematic hardening models.

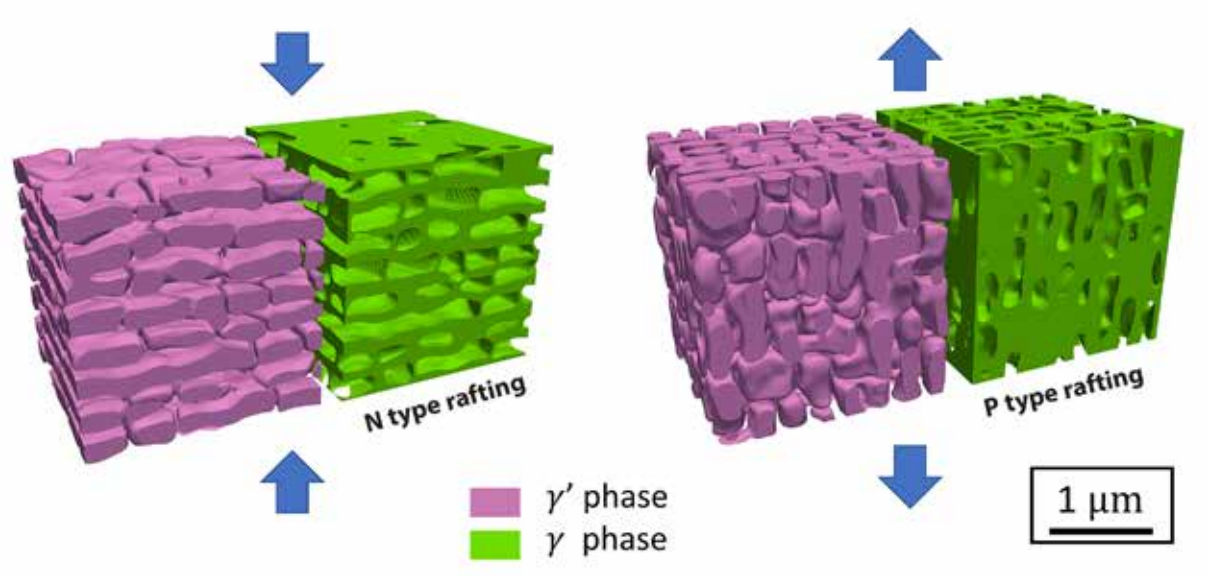


Combined phase-field crystal plasticity simulation of P- and N-type rafting in Co-based superalloys

C. Wang, M. A. Ali, S. Gao, J. V. Görler, I. Steinbach
Acta Materialia, **175**, 21-34 (2019)

We combine a phase-field model with a crystal plasticity model to simulate the microstructural evolution during creep in the Co-based superalloy ERBOCo-2Ta. Three-dimensional simulations of tensile and compressive creep tests in [100] direction were performed to study the rafting behavior in Co-based superalloys. The loss of coherency between γ matrix and γ' precipitate, which is essential for the understanding of rafted structures, is modeled in relation to the dislocation activity in the γ-channels. Special attention is given to the interplay between creep deformation and microstructure stability. Appropriate constitutive modeling is applied to simulate realistic microstructure evolution under creep conditions. Thus, with the removal of the misfit stress, γ' precipitates lose their cuboidal shape and form rafts. During N-type rafting more γ' precipitates coalesce than during P-type rafting. The γ' volume fraction during rafting increases under tensile stress but decreases under compressive stress. The morphological evolution of γ' precipitates under tensile and compressive stresses in Co-based superalloy is consistent with the rafting characteristics in experimental observations.

Phase-field results of N- and P-type rafted microstructure in Co-based superalloys under compressive and tensile load, respectively.



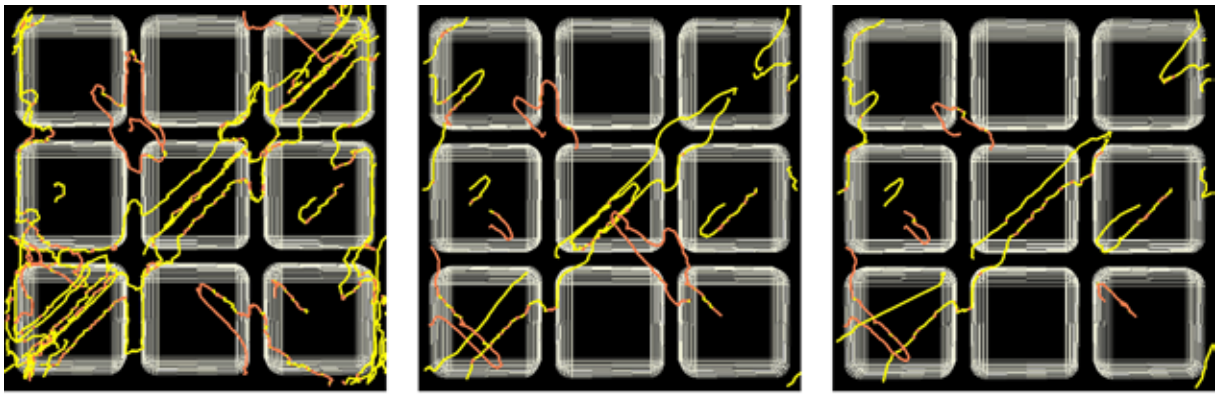
Influence of excess volumes induced by Re and W on dislocation motion and creep in Ni-base single crystal superalloys: A 3D discrete dislocation dynamics study

S. Gao, Z. Yang, M. Grabowski, J. Rogal, R. Drautz, A. Hartmaier

Metals, **9**, 637 (2019)

A comprehensive 3D discrete dislocation dynamics model for Ni-base single crystal superalloys was used to investigate the influence of excess volumes induced by solute atoms Re and W on dislocation motion and creep under different tensile loads at 850 C. The solute atoms were distributed homogeneously only in γ matrix channels. Their excess volumes due to the size difference from the host Ni were calculated by density functional theory. The excess volume affected dislocation glide more strongly than dislocation climb. The relative positions of dislocations and solute atoms determined the magnitude of back stresses on the dislocation motion. Without diffusion of solute atoms, it was found that W with a larger excess volume had a stronger strengthening effect than Re. With increasing concentration of solute atoms, the creep resistance increased. However, a low external stress reduced the influence of different excess volumes and different concentrations on creep.

Dislocation patterns in [101](-1-11) (yellow) and [101](1-1-1) (orange) slip systems in γ matrix channels after 14 s under 200 MPa tensile load along [001] direction at 850 C for different solute atoms. Dislocations are viewed in the projection on (001) crystallographic planes. One dislocation line containing some dislocation jogs with another color indicates the occurrence of dislocation climb: (a) no solute atom; (b) 7 × 10−3 at.% Re; and (c) 7 × 10−3 at.% W.

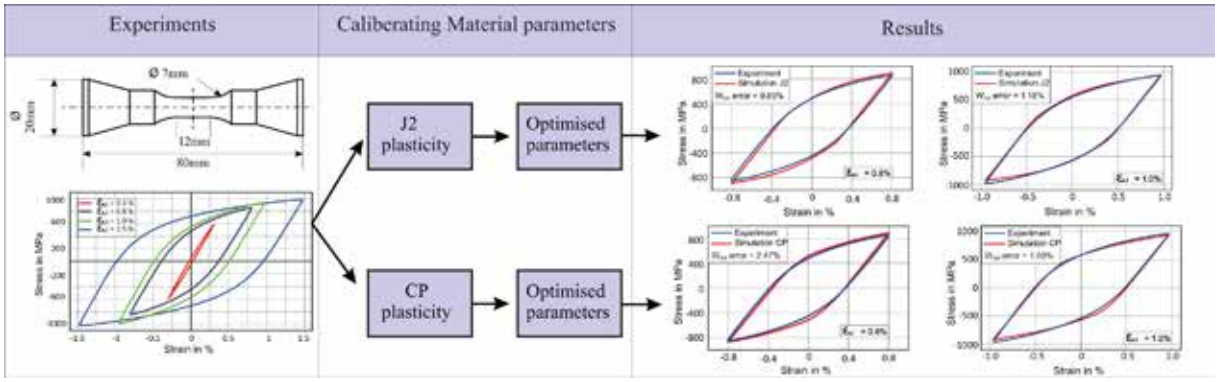


Modelling cyclic behaviour of martensitic steel with J2 plasticity and crystal plasticity

H. Sajjad, S. Hanke, S. Güler , H. u. Hassan, A. Fischer, A. Hartmaier
Journal of Materials MDPI, **12**, 1767 (2019)

In order to capture the stress-strain response of metallic materials under cyclic loading, it is necessary to consider the cyclic hardening behaviour in the constitutive model. Among different cyclic hardening approaches available in the literature, the Chaboche model proves to be very efficient and convenient to model the kinematic hardening and ratcheting behaviour of materials observed during cyclic loading. The purpose of this study is to determine the material parameters of the Chaboche kinematic hardening material model by using isotropic J2 plasticity and micromechanical crystal plasticity (CP) models as constitutive rules in finite element modelling. As model material, we chose a martensitic steel with a very fine microstructure. Thus, it is possible to compare the quality of description between the simpler J2 plasticity and more complex micromechanical material models. The quality of the results is rated based on the quantitative comparison between experimental and numerical stress-strain hysteresis curves for a rather wide range of loading amplitudes. It is seen that the ratcheting effect is captured well by both approaches. Furthermore, the results show that concerning macroscopic properties, J2 plasticity and CP are equally suited to describe cyclic plasticity. However, J2 plasticity is computationally less expensive whereas CP finite element analysis provides insight into local stresses and plastic strains on the microstructural length scale. With this study, we show that a consistent material description on the microstructural and the macroscopic scale is possible, which will enable future scale-bridging applications, by combining both constitutive rules within one single finite element model.

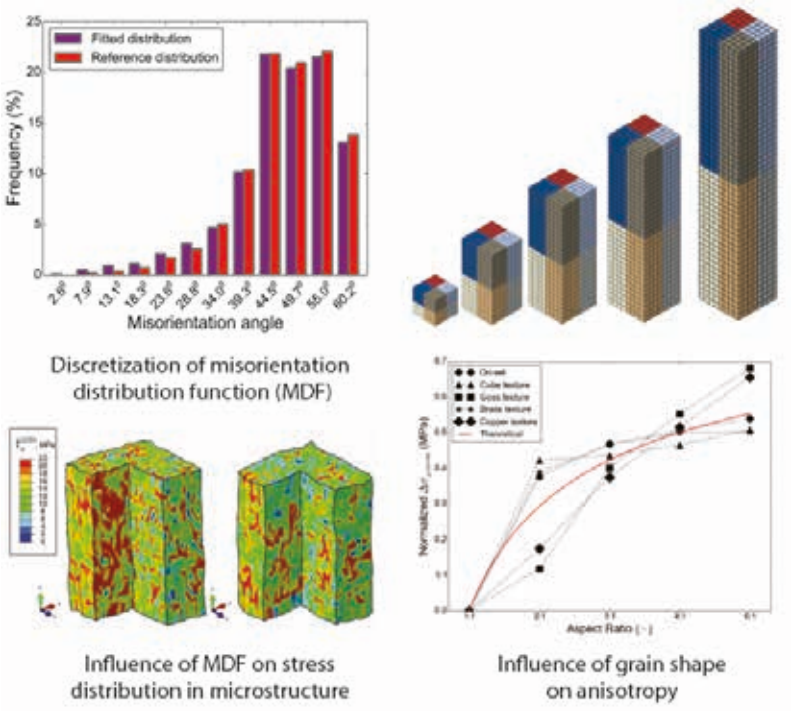
Identification of material parameters using crystal plasticity and J2 plasticity models. An approach towards microstructure sensitive continuum modeling.



Influence of microstructural features on the strain hardening behavior of additively manufactured metallic components

A. Biswas, M. R. G. Prasad, N. Vajragupta, H. u. Hassan, F. Brenne, T. Niendorf, A. Hartmaier, V. Prasad
Advanced Engineering Materials, **21**, 1900275 (2019)

I Additive Manufacturing (AM) has recently become one of the key manufacturing processes in the era of Industry 4.0 because of its highly flexible production scheme. Due to complex thermal cycles during the manufacturing process itself and special solidification conditions, the microstructure of AM components often exhibits elongated grains together with a pronounced texture. These microstructural features significantly contribute to an anisotropic mechanical behavior. In this work, the microstructure and mechanical properties of additively manufactured samples of 316L stainless steel are characterized experimentally and a micromechanical modeling approach is employed to predict the macroscopic properties. The objective of this work is to study the effects of texture and microstructural morphology on yield strength and strain hardening behavior of face-centered cubic additively manufactured metallic components. To incorporate the texture in synthetic Representative Volume Elements (RVE), the proposed approach considers both the crystallographic and grain boundary textures. The mechanical behavior of these RVEs is modeled using crystal plasticity finite element method, which incorporates size effects through the implementation of strain gradients.



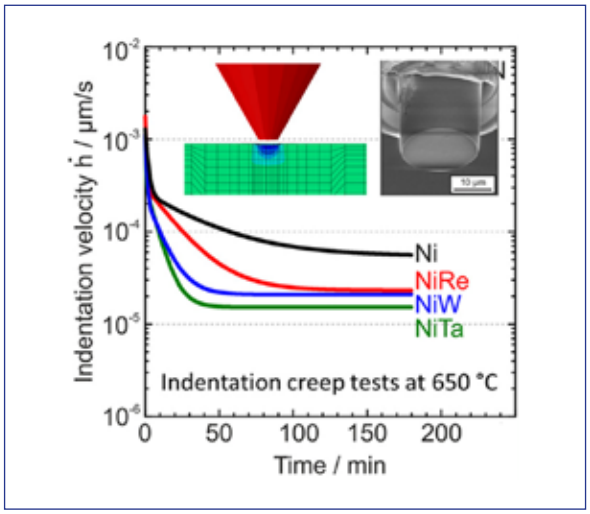
A method for fitting the disorientation distribution function (MDF) together with its applications to study the influence of MDF on stress distribution in the microstructure and investigation of the grain shape effect.

New flat-punch indentation creep testing approach for characterizing the local creep properties at high temperatures

D. Matschkal-Amberger, M. Kolb, S. Neumeier, S. Gao, A. Hartmaier, K. Durst, M. Göken

Materials & Design, **183**, 108090 (2019)

An indentation creep testing approach has been developed which allows measuring creep properties at high temperatures. In contrast to existing indentation or impression creep experiments, the approach described here allows to achieve a quite high spatial resolution, as flat punch indenters with a diameter of only 20 µm are used. First indentation creep tests have been performed on single crystalline nickel and nickel binary solid solution alloys with Re, Ta or W as alloying elements, respectively. The indentation creep tests have been carried out at a temperature of 650 °C and stress levels in the range of 85 to 400 MPa. Using crystal plasticity finite element modeling, the indentation creep response is converted into equivalent uniaxial creep properties. It is shown that the conversion parameters, evaluated for differently oriented single crystals, can be chosen independently of the creep rate exponent in the power law creep regime. It is found that the indentation creep results agree well with conventional uniaxial creep tests. Furthermore, the results show that Ta is the most effective solid solution strengthener of all tested solid-solution strengtheners at 650 °C because of the large atomic size mismatch, followed by W and Re.

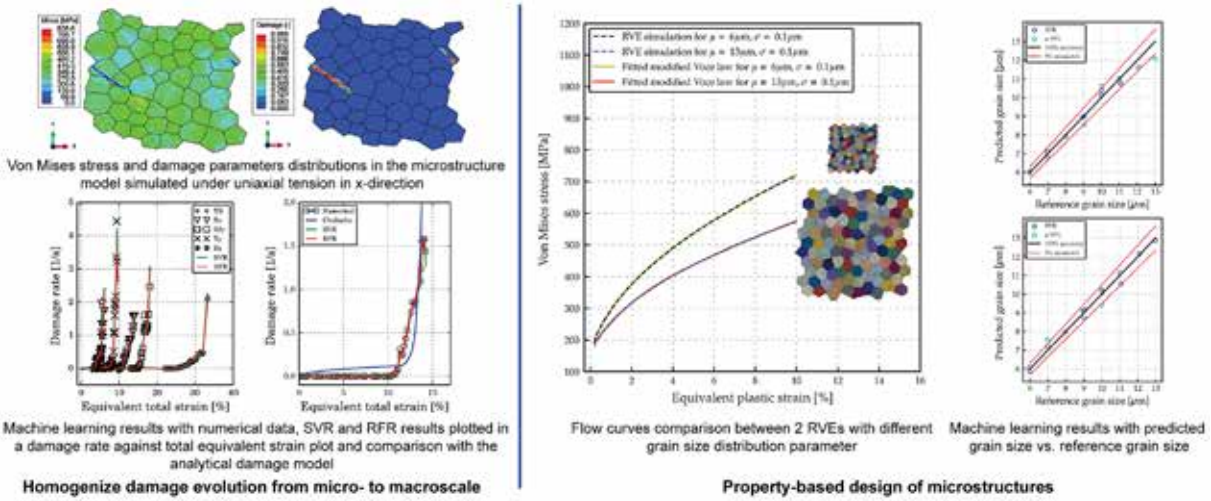


FE stress field simulation, cylindrical flat punch indenter tip, and indentation creep curves of different Ni solid solutions.

Modeling macroscopic material behavior with machine learning algorithms trained by micromechanical simulations

D. Reimann, K. Nidadavolu, H. u. Hassan, N. Vajragupta, T. Glasmachers, P. Junker, A. Hartmaier
Frontiers in Materials, **6**, 181 (2019)

Micromechanical modeling of material behavior has become an accepted approach to describe the macroscopic mechanical properties of polycrystalline materials in a microstructure-sensitive way. The microstructure is modeled by a representative volume element (RVE), and the anisotropic mechanical behavior of individual grains is described by a crystal plasticity model. Such micromechanical models are subjected to mechanical loads in a finite element (FE) simulation and their macroscopic behavior is obtained from a homogenization procedure. However, such micromechanical simulations with a discrete representation of the material microstructure are computationally very expensive, in particular when conducted for 3D models, such that it is prohibitive to apply them for process simulations of macroscopic components. In this work, we suggest a new approach to develop microstructure-sensitive, yet flexible and numerically efficient macroscopic material models by using micromechanical simulations for training Machine Learning (ML) algorithms to capture the mechanical response of various microstructures under different loads. In this way, the trained ML algorithms represent a new macroscopic constitutive relation, which is demonstrated here for the case of damage modeling. In a second application of the combination of ML algorithms and micromechanical modeling, a proof of concept is presented for the application of trained ML algorithms for microstructure design with respect to desired mechanical properties. The input data consist of different stress-strain curves obtained from micromechanical simulations of uniaxial testing of a wide range of microstructures. The trained ML algorithm is then used to suggest grain size distributions, grain morphologies and crystallographic textures, which yield the desired mechanical response for a given application. For validation purposes, the resulting grain microstructure parameters are used to generate RVEs, accordingly and the macroscopic stress-strain curves for those microstructures are calculated and compared with the target quantities. The two examples presented in this work, demonstrate clearly that ML methods can be trained by micromechanical simulations, which capture material behavior and its relation to microstructural mechanisms in a physically sound way. Since the quality of the ML algorithms is only as good as that of the micromechanical model, it is essential to validate these models properly. Furthermore, this approach allows a hybridization of experimental and numerical data.



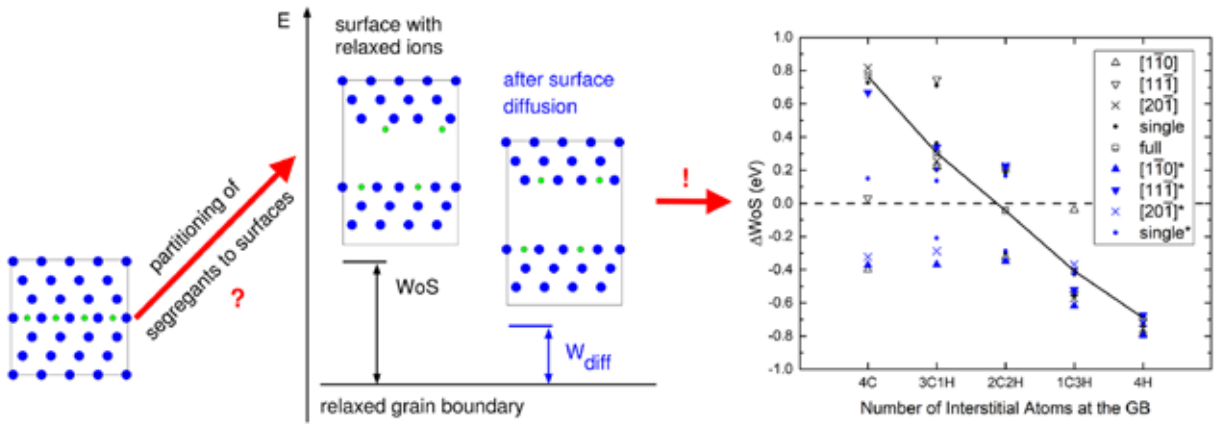
Two applications of machine learning algortihms trained by micromechanical simulations.

Partitioning of interstitial segregants during decohesion: A DFT case study of the Σ3 symmetric tilt grain boundary in ferritic steel

X. Huang, R. Janisch

Materials, **12**, 2971 (2019)

The effect of hydrogen atoms at grain boundaries in metals is usually detrimental to the cohesion of the interface. This effect can be quantified in terms of the strengthening energy, which is obtained following the thermodynamic model of Rice and Wang. A critical component of this model is the bonding or solution energy of the atoms to the free surfaces that are created during decohesion. At a grain boundary in a multicomponent system, it is not immediately clear how the different species would partition and distribute on the cleaved free surfaces. In this work, it is demonstrated that the choice of partitioning pattern has a significant effect on the predicted influence of H and C on grain boundary cohesion. To this end, the Σ3(112)[110] symmetric tilt grain boundary in bcc Fe with different contents of interstitial C and H was studied, taking into account all possible distributions of the elements, as well as surface diffusion effects. H as a single element has a negative influence on grain boundary cohesion, independent of the details of the H distribution. C, on the other hand, can act both ways, enhancing or reducing the cohesion of the interface. The effect of mixed H and C compositions depends on the partition pattern. However, the general trend is that the number of detrimental cases increases with increasing H content. A decomposition of the strengthening energy into chemical and mechanical contributions shows that the elastic contribution dominates at high C contents, while the chemical contribution sets the trend for high H contents.



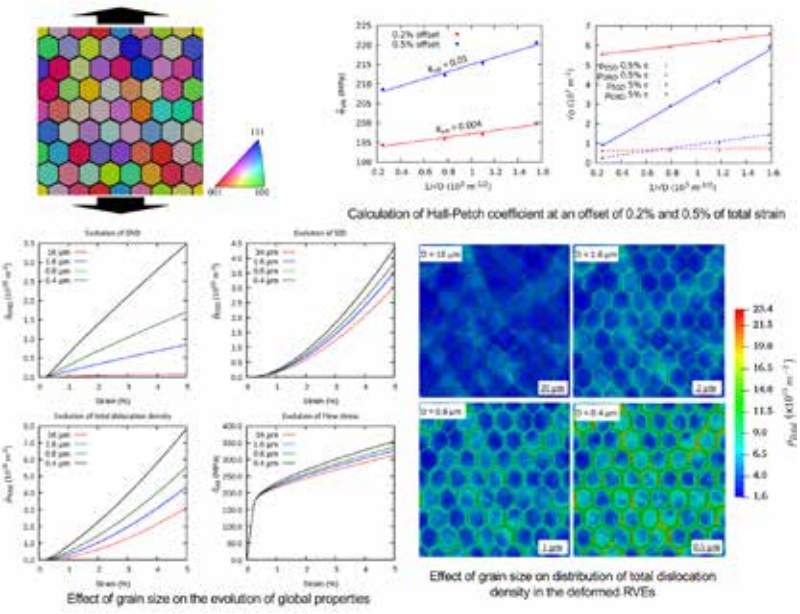
Different surface distributions of segregating elements during separation lead to a different effect on cohesion.

Studying grain boundary strengthening by dislocation-based strain gradient crystal plasticity coupled with a multi-phase-field model

W. Amin, M. A. Ali, N. Vajragupta, A. Hartmaier

Materials, **12**, 2977 (2019)

One ambitious objective of Integrated Computational Materials Engineering (ICME) is to shorten the materials development cycle by using computational materials simulation techniques at different length scales. In this regard, the most important aspects are the prediction of the microstructural evolution during material processing and the understanding of the contributions of microstructural features to the mechanical response of the materials. One possible solution to such a challenge is to apply the Phase Field (PF) method because it can predict the microstructural evolution under the influence of different internal or external stimuli, including deformation. To accomplish this, it is necessary to take into account plasticity or, specifically, non-homogeneous plastic deformation, which is particularly important for investigating the size effects in materials emerging at the micron length scale. In this work, we present quasi-2D simulations of plastic deformation in a face centred cubic system using a finite strain formulation. Our model consists of dislocation-based strain gradient crystal plasticity implemented into a PF code. We apply this model to study the influence of grain size on the mechanical behavior of polycrystals, which includes dislocation storage and annihilation. Furthermore, the initial state of the material before deformation is also considered. The results show that a dislocation-based strain gradient crystal plasticity model can capture the Hall-Petch effect in many aspects. The model reproduced the correct functional dependence of the flow stress of the polycrystal on grain size without assigning any special properties to the grain boundaries. However, the predicted Hall-Petch coefficients are significantly smaller than those found typically in experiments. In any case, we found a good qualitative agreement between our findings and experimental results.

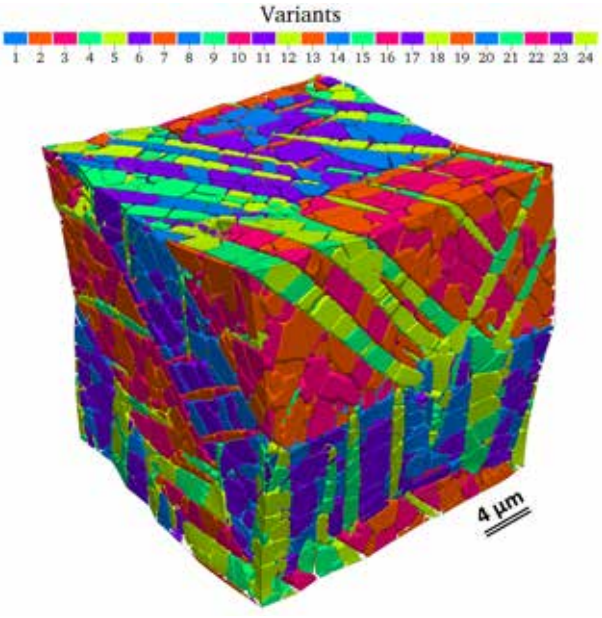


Phase-field model of grain boundary strengthening. The mechanical behavior of a polycrystal is investigated with a dislocation-density-based crystal plasticity method that has been implemented into the ICAMS phase-field code OpenPhase. With this model the role of dislocation pile-ups at grain boundaries during plastic deformation and the resulting strengthening effect have been analyzed.

Phase-field simulation of martensite microstructure in low-carbon steel

O. Shchyglo, G. Du, J. K. Engels, I. Steinbach
Acta Materialia, **175**,415-425 (2019)

We present three-dimensional phase-field simulations of martensite microstructure formation in low-carbon steel. In this study, a full set of 24 Kurdjumov-Sachs symmetry variants of martensite is considered. Three different carbon compositions are investigated in order to reveal the effect of carbon content on the martensite microstructure formation. The simulations are performed using the finite strain framework which allows considering real martensite transformation strains. Using Neuber elasto-plastic approximation to the mechanical equilibrium solution, realistic stresses and strains can be obtained during martensite formation resulting in realistic mechanical driving forces for the transformation. The simulated microstructures are compared to experimental results for three carbon compositions. Good agreement between simulated and experimental results is achieved.



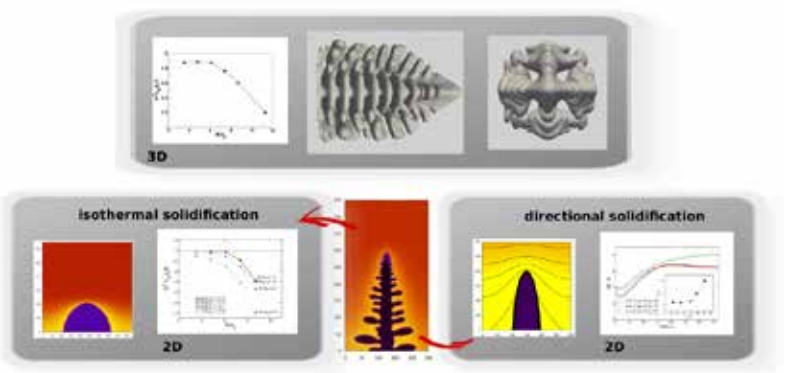
Simulated martensite microstructure in low carbon steel consisting of 24 Kurdjumov-Sachs symmetry variants.

Comparative study of different anisotropy and potential formulations of phase-field models for dendritic solidification

J. Kundin, I. Steinbach
Computational Materials Science, **170**,109197 (2019)

Phase-field model formulations with double well and double obstacle potentials, and different anisotropy models are investigated with respect to their potential to simulate (i) tip growth on a quantitative level, (ii) well resolved side-branching. The dilute binary alloy Al-4 at%Cu is used as a model alloy. The effects of the numerical re- solution (the ratio of the capillary length to the grid spacing) on the growth velocity are studied by means of convergence tests for isothermal and directional solidification in comparison to the theoretical values calculated by the Green-function method (A. Karma, W.J. Rappel, Phys. Rev. E 57 (1998) 4323). An interface stability parameter is introduced as a measure for the estimation of the maximum value of the grid spacing for effective simulations. We show that predominantly the side-branching occurs at numerical resolution lower than the limit value needed to produce correct results in accordance to the convergence analysis. The best results for dendrite growth at a relevant numerical resolution are obtained for the double well potential.

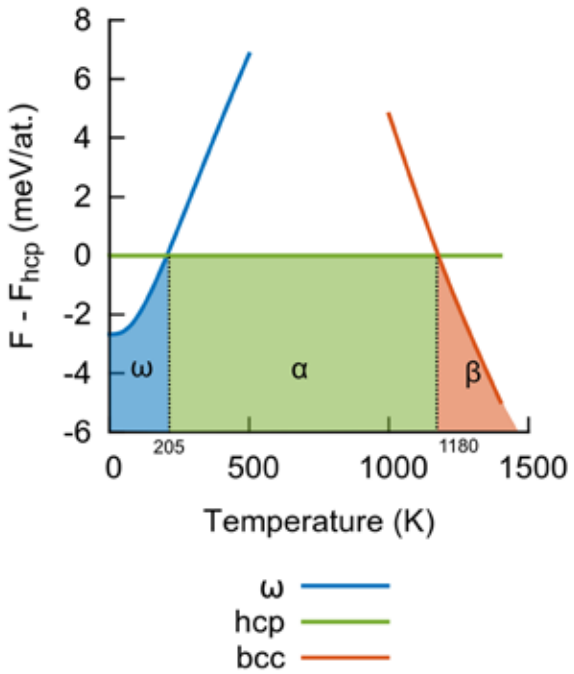
Phase-field models for dentritic solidification.



Phase transitions in titanium with an analytic bond-order potential

A. Ferrari, M. F. Schröder, Y. Lysogorskiy, J. Rogal, M. Mrovec, R. Drautz
Modelling and Simulation in Materials Science and Engineering, **27**, 85008 (2019)

Titanium is the base material for a number of technologically important alloys for energy conversion and structural applications. Atomic-scale studies of Ti-based metals employing first-principles methods, such as density functional theory, are limited to ensembles of a few hundred atoms. To perform large-scale and/or finite temperature simulations, computationally more efficient interatomic potentials are required. In this work, we coarse grain the tight-binding (TB) approximation to the electronic structure and develop an analytic bond-order potential (BOP) for Ti by fitting to the energies and forces of elementary deformations of simple structures. The BOP predicts the structural properties of the stable and defective phases of Ti with a quality comparable to previous TB parameterizations at a much lower computational cost. The predictive power of the model is demonstrated for simulations of martensitic transformations.



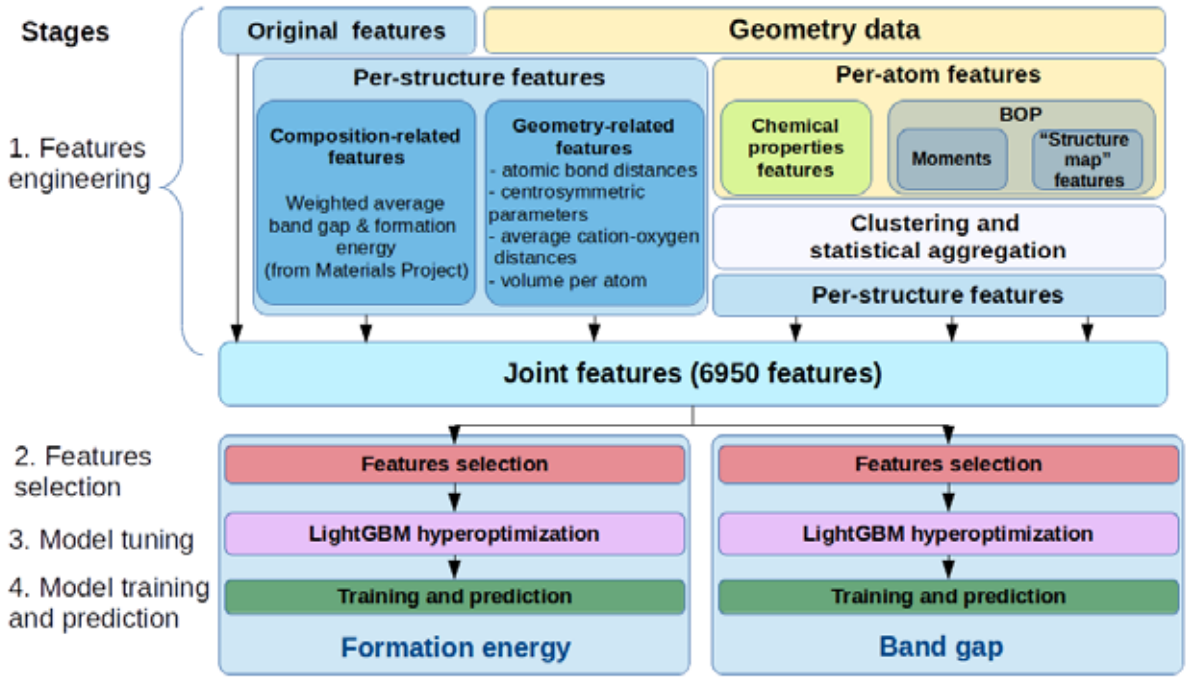
Helmholtz free energy differences for titanium bulk phases (w.r.t. the hcp phase) as a function of temperature.

Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition

C. Sutton, L. M. Ghiringhelli, T. Yamamoto, Y. Lysogorskiy, L. Blumenthal, T. Hammerschmidt, J. R. Golebiowski, X. Liu, A. Ziletti, M. Scheffler

npj Computational Materials, **5**, 111 (2019)

A public data-analytics competition was organized by the Novel Materials Discovery (NOMAD) Centre of Excellence and hosted by the online platform Kaggle by using a dataset of 3,000 (Al x Ga y In 1–x–y) 2 O 3 compounds. Its aim was to identify the best machine-learning (ML) model for the prediction of two key physical properties that are relevant for optoelectronic applications: the electronic bandgap energy and the crystalline formation energy. Here, we present a summary of the top-three ranked ML approaches. The first-place solution was based on a crystal-graph representation that is novel for the ML of properties of materials. The second-place model combined many candidate descriptors from a set of compositional, atomic-environment-based, and average structural properties with the light gradient-boosting machine regression model. The third-place model employed the smooth overlap of atomic position representation with a neural network. The Pearson correlation among the prediction errors of nine ML models (obtained by combining the top-three ranked representations with all three employed regression models) was examined by using the Pearson correlation to gain insight into whether the representation or the regression model determines the overall model performance. Ensembling relatively decorrelated models (based on the Pearson correlation) leads to an even higher prediction accuracy.

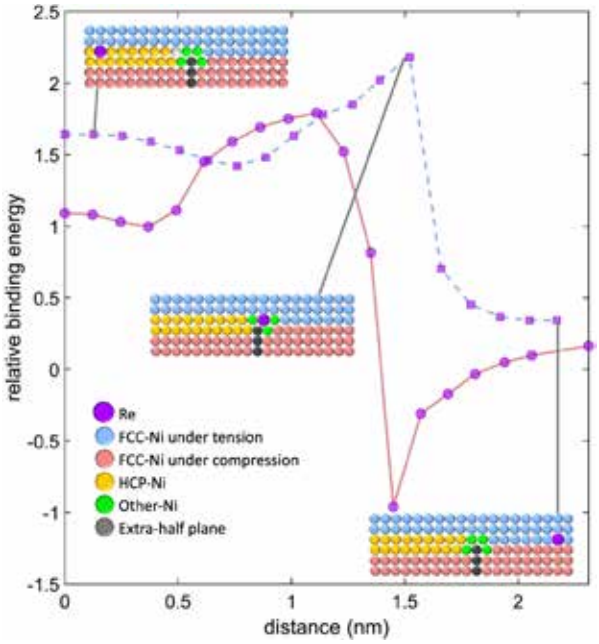


Architecture of the machine-learning model that reached the second place in the NOMAD 2018 Kaggle competition on predicting the formation energy and the band gap of Al-Ga-In-O compounds for optoelectronic applications.

Imaging individual solute atoms at crystalline imperfections in metals

S. Katnagallu, L. T. Stephenson, I. Mouton, C. Freysoldt, A. P. Subramanyam, J. Jenke, A. C. Ladines, S. Neumeier, T. Hammerschmidt, R. Drautz, J. Neugebauer, F. Vurpillot, D. Raabe, B. Gault
New Journal of Physics, **21**, 123020 (2019)

Directly imaging all atoms constituting a material and, maybe more importantly, crystalline defects that dictate materials' properties, remains a formidable challenge. Here, we propose a new approach to chemistry-sensitive field-ion microscopy (FIM) combining FIM with time-of-flight mass-spectrometry (tof-ms). Elemental identification and correlation to FIM images enabled by data mining of combined tof-ms delivers a truly analytical-FIM (A-FIM). Contrast variations due to different chemistries is also interpreted from density-functional theory (DFT). A-FIM has true atomic resolution and we demonstrate how the technique can reveal the presence of individual solute atoms at specific positions in the microstructure. The performance of this new technique is showcased in revealing individual Re atoms at crystalline defects formed in Ni–Re binary alloy during creep deformation. The atomistic details offered by A-FIM allowed us to directly compare our results with simulations, and to tackle a long-standing question of how Re extends lifetime of Ni-based superalloys in service at high-temperature.



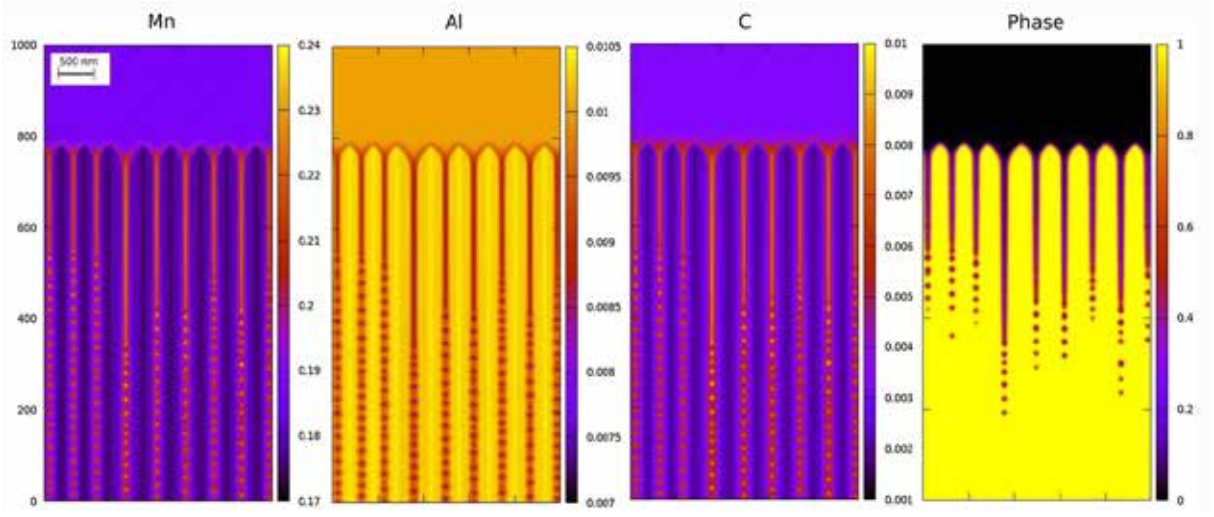
Interaction of Re solute atom with edge dislocation in Ni as obtained by tight-binding calculations (available via license CC-BY 3.0).

Microstructure evolution of binary and multicomponent manganese steels during selective laser melting: phase-field modeling and experimental validation

J. Kundin, A. Ramazani, U. Prahl, C. Haase

Metallurgical and Materials Transactions A, **50**, 2022-2040 (2019)

In additive manufacturing processes, solidification velocities are extremely high in comparison to ordinary directional solidification. Therefore, the dependencies of the primary dendrite arm spacing (PDAS) on the process parameters deviate from the dependencies predicted by standard analytical methods. In this work, we investigate the microstructure evolution and element distribution in Fe-18.9Mn and Fe-18.5Mn-Al-C alloys solidified during the selective laser melting process. A quantitative multicomponent phase-field model verified by Green-function calculations (Karma, Rappel: Phys. Rev. E, 1998, 57, 4323) and the convergence analysis is used. The resulting non-standard dependencies of the PDAS on the process parameters in a wide range of solidification velocities are compared with analytical calculations. It is shown that the numerical values of the PDAS are similar to the values predicted by the Kurz–Fisher method for the low and intermediate solidification velocities and are smaller for the solidification velocities higher than 0.03 m/s. The PDAS and the Mn distribution in a Fe-18.5Mn-Al-C alloy are compared to the experimental results and a very good agreement is found.

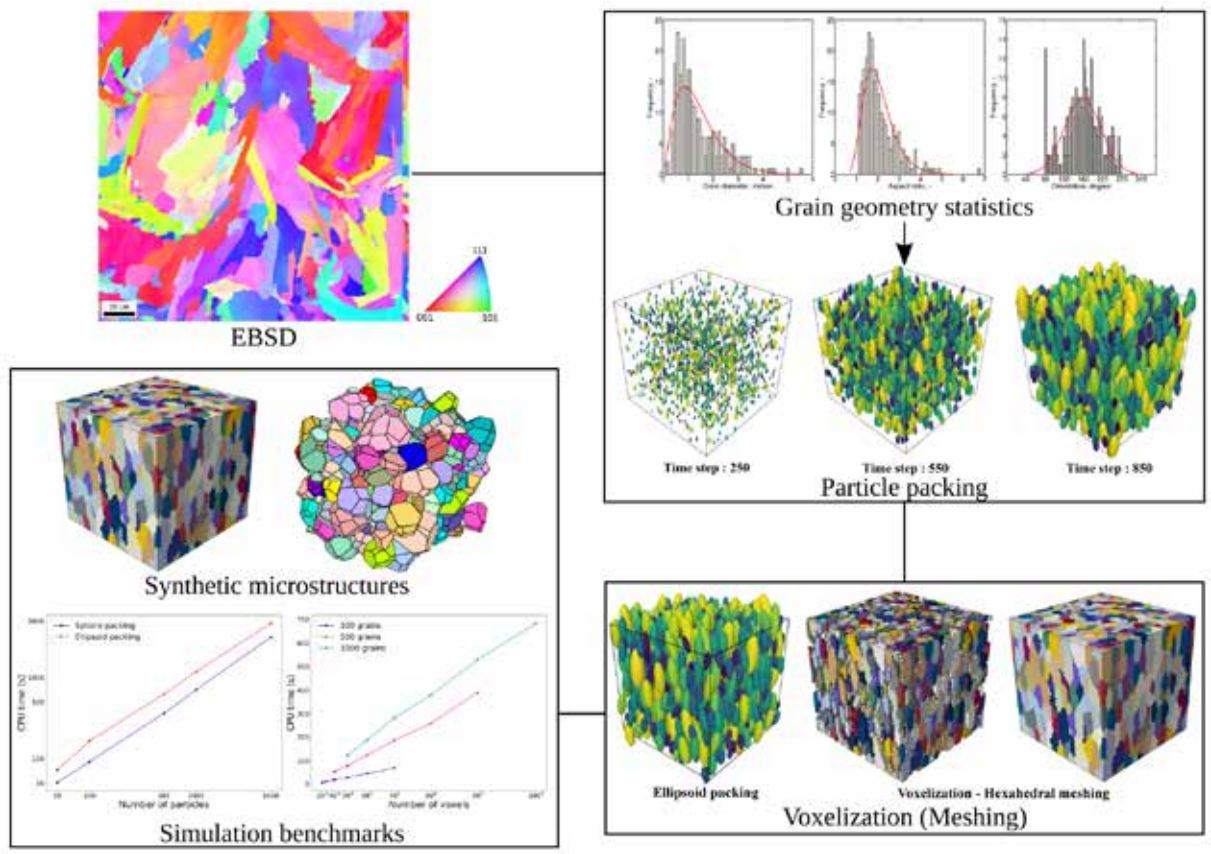


Microstructure evolution of the Fe-18.5Mn-Al-C alloy during SLM. The temperature gradient 4.6 x 10 6 K/m and the cooling rate 3 x 10 5 K/s. The concentration fields of Mn, Al, C are shown in mass fractions.

Kanapy:
A Python package for generating complex synthetic polycrystalline microstructures

M. Ramaswamy Guru Prasad, N. Vajragupta, A. Hartmaier
Journal of Open Source Software, **4**, 1732 (2019)

Kanapy is a Python package for generating complex synthetic polycrystalline microstructures based on the collision driven particle dynamics approach. Kanapy is designed to model irregular shaped grains and developed to provide an alternative to the existing particle packing approach, the RSA technique. This addresses the limitations of the existing microstructure generation techniques described earlier. In this regard, Kanapy employs a two-layer collision detection scheme, wherein the outer layer utilizes an octree spatial partitioning data structure to estimate which particles should be checked for collision. The inner layer consists of a bounding spheres hierarchy, which carries out the collision detection only if the bounding spheres between two particles overlap. The computational complexity involved in using the octree data structure is of the order O(nlog(n)). The actual collision detection between two static ellipsoidal particles is determined by employing the algebraic separation condition developed by Wang et al. (2001). Using the built-in voxelization routine, complex microstructures like those found in additively manufactured components can be easily created.



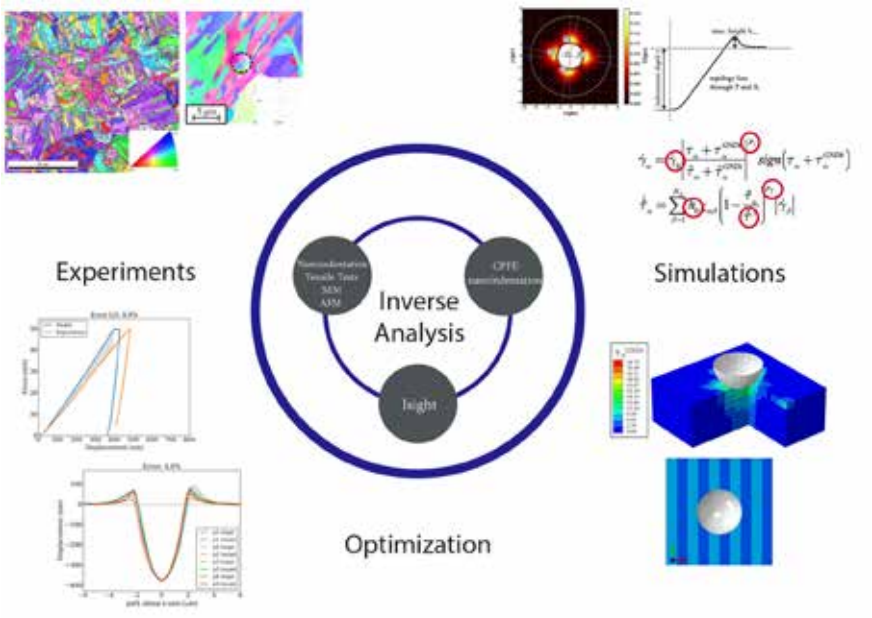
Synthetic microstructure generator - Kanapy.

Parameterization of a non-local crystal plasticity model for tempered lath martensite using nanoindentation and inverse method

J. K. Engels, N. Vajragupta, A. Hartmaier
Frontiers in Materials, **6**, 247 (2019)

Crystal plasticity (CP) models have proven to accurately describe elasto-plastic behavior on micro- and nanometer length scales in numerous applications. However, their parameterization requires a series of experiments and inverse analysis of the results. In this regard, nanoindentation promises to be a well-suited tool for realizing a parameterization approach to determine all model parameters. The objective of this work is to develop a parameterization technique for a non-local CP model by means of an accessible and reproducible workflow. To determine its feasibility, tempered lath martensite with two different carbon contents is used as testing material. The workflow combines nanoindentation tests with finite element simulations. First, indentation into single packets of tempered lath martensitic specimen is yielding the load-displacement curves and the residual imprint topology on the surface with the help of atomic force microscopy. In a second step, a finite element simulation of the indentation using non-local crystal plasticity as constitutive model is performed with estimated model parameters. In the next step, non-local CP parameters are systematically adapted in an optimization scheme to reach optimal agreement with experiments. As a final validation step, it is successfully demonstrated that the CP model parameterized by nanoindentation is able to determine the macroscopic stress-strain response of polycrystals. Two observations are made: on the one hand, the material properties locally scatter very strongly, which is caused by fluctuations in microstructure and chemistry. On the other hand, a novel method has been demonstrated, were an inverse analysis is used to parameterize a non-local CP model for highly complex microstructures as those of tempered lath martensite. The novelty of this study is the application of nanoindentation and optimization scheme to parameterize a higher-order CP model of oligocrystals with a complex microstructure like the tempered lath martensite as well as the topology identification method developed and employed for both experiment and numerics.

The workflow for parameterisation of the non-local crystal plasticity model of the tempered lath martensite by using nanoindentation test and inverse method.



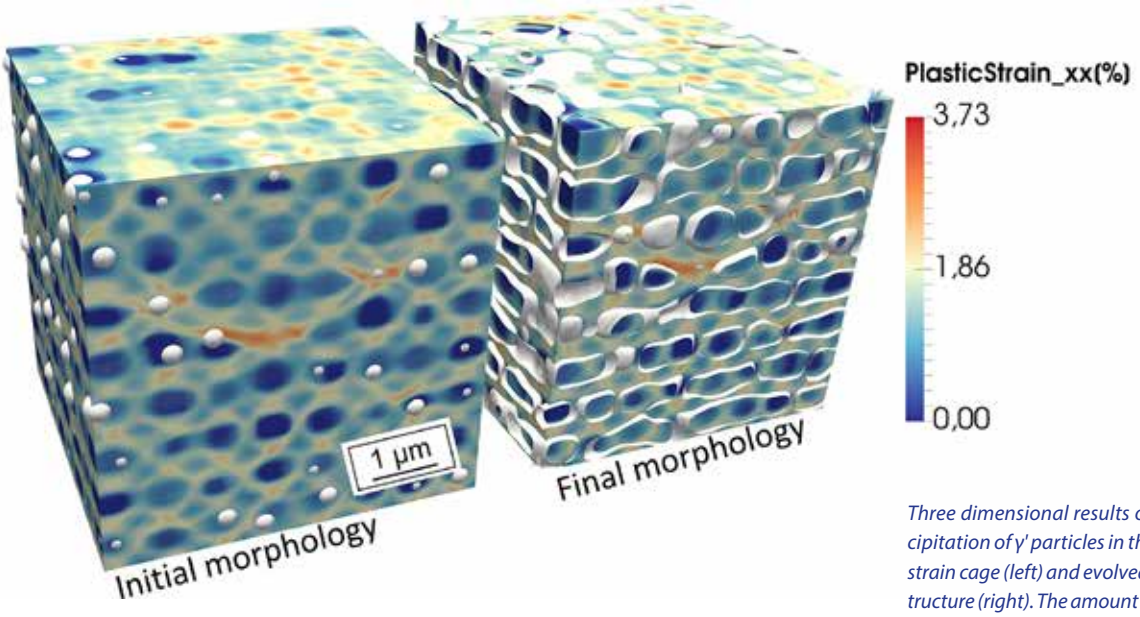
15. Research Highlights

2020

Role of coherency loss on rafting behavior of Ni-based superalloys

M. A. Ali, J. V. Görler, I. Steinbach

Computational Materials Science, **171**, 109279 (2020)



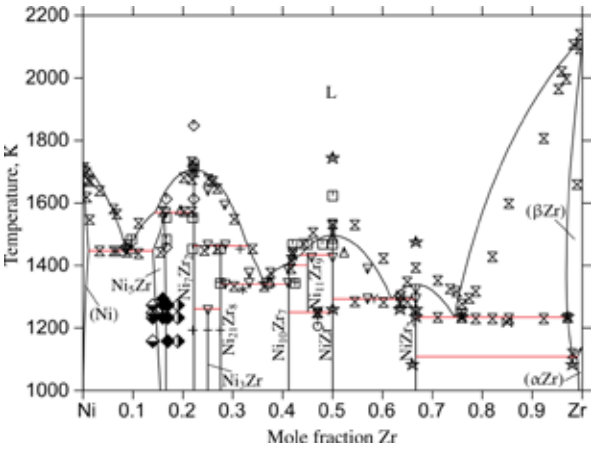
Three dimensional results of re-precipitation of γ' particles in the plastic strain cage (left) and evolved microstructure (right). The amount of plastic strain is displayed in the matrix and γ' is being in white color.

The role of coherency loss on rafting of superalloys under high temperature low stress creep conditions is investigated by phase-field crystal plasticity simulations. It is demonstrated that coalescence, critically depending on the state of coherency between precipitate and matrix is crucial to understand the rafting behavior of superalloys. An explicit mechanisms is developed predicting coherency loss based on the plastic activity in the matrix. The simulations are verified using experimental creep test results.

Thermodynamic modelling of the Ni–Zr system

A. Jana, S. Sridar, S. G. Fries, T. Hammerschmidt, H. K. Kumar
Intermetallics, **116**, 106640 (2020)

In this work, we report the thermodynamic modelling of the Ni–Zr system using the Calphad method combined with ab initio calculations. Density functional theory (DFT) is employed to calculate the enthalpy of formation of the intermediate phases. The calculated enthalpies of formation are in close agreement with the experimental data. An approach based on special quasirandom structures (SQS) was used for calculating the enthalpy of mixing of the fcc solid solution. The vibrational contribution to the heat capacities of NiZr, $NiZr_2$, Ni_3Zr and Ni_7Zr_2 phases were calculated using the quasiharmonic approximation (QHA) and the corresponding electronic contribution was obtained using an approach based on Mermin statistics. The total heat capacities for these phases were fitted to appropriate expressions and integrated to obtain the Gibbs energy functions valid down to 0 K. The calculated thermochemical properties along with critically selected experimental constitutional and thermochemical data served as input for the thermodynamic optimisation of the system. The calculated phase equilibria and the thermodynamic properties using the optimised Gibbs energy functions are in good agreement with the input data. The calculated congruent melting points of NiZr and $NiZr_2$ phases are close to the recent experimental data. The $Ni_{10}Zr_7$ phase forms by a peritectic reaction, which is also in agreement with the experimental data.



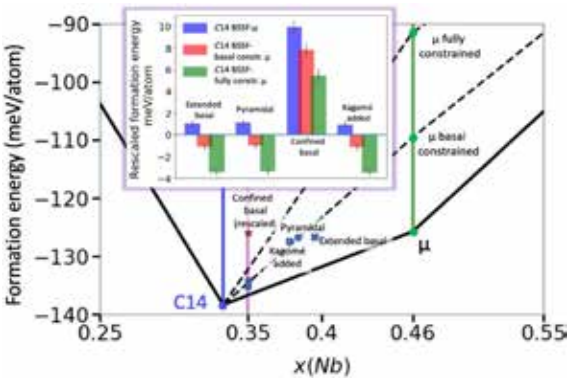
Phase equilibrium in the Ni-Zr system obtained by thermodynamic modelling using experimental data and ab initio calculations.

Atomic scale configuration of planar defects in the Nb-rich C14 Laves phase $NbFe_2$

M. Slapakova, A. Zendegani, C. Liebscher, T. Hickel, J. Neugebauer, T. Hammerschmidt, A. Ormeci, J. Grin, G. Dehm, K. S. Kumar, F. Stein
Acta Materialia, **183**, 362-376 (2020)

Laves phases belong to the group of tetrahedrally close-packed intermetallic phases, and their crystal structure can be described by discrete layer arrangements. They often possess extended homogeneity ranges and the general notion is that deviations from stoichiometry are accommodated by anti-site atoms or vacancies. The present work shows that excess Nb atoms in a Nb-rich $NbFe_2$ C14 Laves phase can also be incorporated in various types of planar defects. Aberration-corrected scanning transmission electron microscopy and density functional theory calculations are employed to characterize the atomic configuration of these defects and to establish stability criteria for them. The planar defects can be categorized as extended or confined ones. The extended defects lie parallel to the basal plane of the surrounding C14 Laves phase and are fully coherent. They contain the characteristic Zr_4Al_3-type (O) units found in the neighboring Nb_6Fe_7 μ phase. An analysis of the chemical bonding reveals that the local reduction of the charge transfer is a possible reason for the preference of this atomic arrangement. However, the overall layer stacking deviates from that of the perfect μ phase. The ab initio calculations establish why these exceptionally layered defects can be more stable configurations than coherent nano-precipitates of the perfect μ phase. The confined defects are observed

with pyramidal and basal habit planes. The pyramidal defect is only ~1 nm thick and resembles the perfect μ phase. In contrast, the confined basal defect can be regarded as only one single O unit and it appears as if the stacking sequence is disrupted. This configuration is confirmed by ab initio calculations to be metastable.

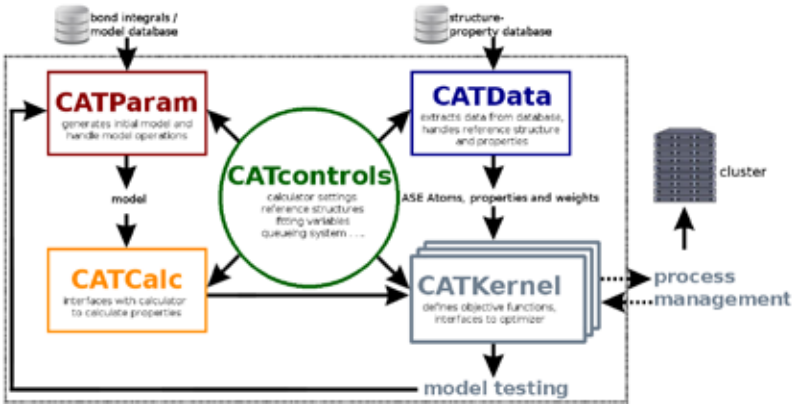


Formation energy of experimentally observed defect structures as obtained by density-functional theory calculations in the convex hull diagram of the Fe-Nb system.

BOPcat software package for the construction and testing of tight-binding models and bond-order potentials

A. C. Ladines, T. Hammerschmidt, R. Drautz
Computational Materials Science, **173**, 109455 (2020)

Atomistic models like tight-binding (TB), bond-order potentials (BOP) and classical potentials describe the interatomic interaction in terms of mathematical functions with parameters that need to be adjusted for a particular material. The procedures for constructing TB/BOP models differ from the ones for classical potentials. We developed the BOPcat software package as a modular python code for the construction and testing of TB/BOP parameterizations. It makes use of atomic energies, forces and stresses obtained by TB/BOP calculations with the BOPfox software package. It provides a graphical user interface and flexible control of raw reference data, of derived reference data like defect energies, of automated construction and testing protocols, and of parallel execution in queuing systems. We demonstrate the concepts and usage of the BOPcat software and illustrate its key capabilities by exemplary constructing and testing a parameterization of a magnetic BOP for Fe. We provide a parameterization protocol with a successively increasing set of reference data that leads to good transferability to a variety of properties of the ferromagnetic bcc groundstate and to crystal structures which were not part of the training set.

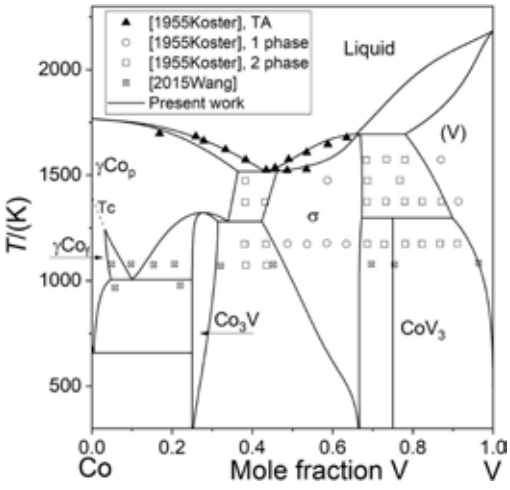


Workflow of constructing and testing of tight-binding models and analytic bond-order potentials with the BOPcat software package.

Structural stability of Co–V intermetallic phases and thermodynamic description of the Co–V system

P. Wang, T. Hammerschmidt, U. R. Kattner, G. B. Olson
Calphad, **68**, 101729 (2020)

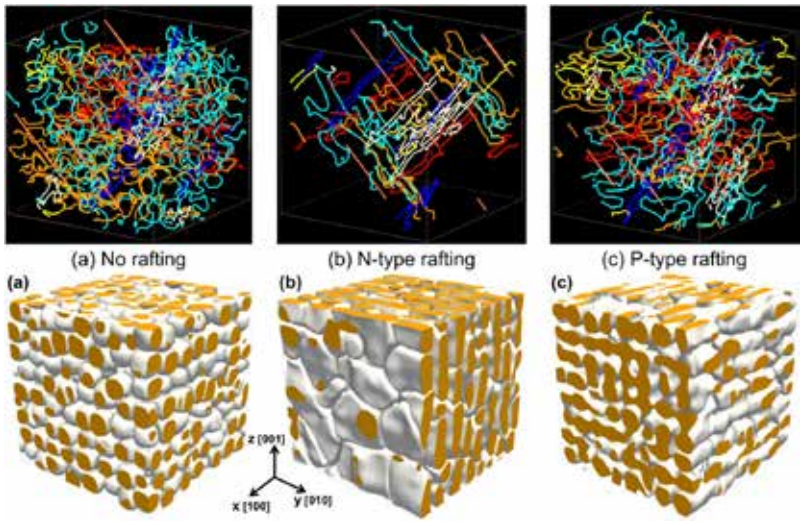
The Co-V system has been reviewed. Density functional theory (DFT) calculations using the generalized gradient approximation (GGA) were used to obtain the energies for the end-members for all three intermediate phases, Co3V, σ and CoV3. Results from DFT calculations considering spin polarization were used to evaluate the CALPHAD (Calculation of phase diagrams) model parameters. The method to evaluate the contribution of the magnetism to the energies of Co-rich compounds that was introduced in our previous work is presented in more detail in the present work. For the description of the σ phase, the magnetic part of the total energy is included in the description of the pure Co end-member compound resulting in a non-linear description of the magnetic contribution over composition. The calculated phase diagram obtained from the present CALPHAD description is in good agreement with the experimental data. The metastable FCC-L12 phase diagram was calculated and compared with experimental data.



Phase diagram of Co-V based on ab-initio calculations and comparison to experimental data.

Influence of rafted microstructures on creep in Ni-base single crystal superalloys: A 3D discrete dislocation dynamics study

S. Gao, M. A. Ali, A. Hartmaier
Modelling and Simulation in Materials Science and Engineering, **28**, 25001 (2020)



Dislocation configurations in different microstructures in 80 ns creep deformation under 350 MPa tensile load along [100] direction at 950 °C. RVE is generated by Phase Field method.

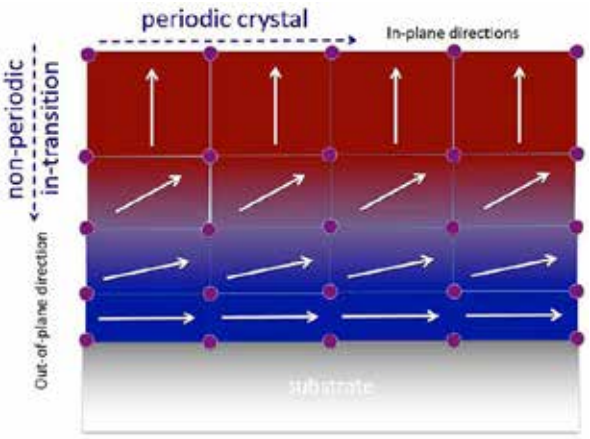
Ni-base single-crystal superalloys exhibit a dynamic evolution of their microstructure during operation at elevated temperatures. The rafting of γ′ precipitates changes the mechanical behavior in a way that was understood insufficiently. In this work, we combine a phase-field method with a discrete dislocation dynamics model to clarify the influence of different rafted microstructures with the same initial dislocation density and configuration on creep behavior. The unrafted and rafted microstructures of Ni-base single crystal superalloys are simulated by a phase-field crystal plasticity method. By introducing these microstructures into a 3D discrete dislocation dynamics (DDD) model, the creep behavior under uniaxial loads of 350 and 250 MPa along [100] direction at 950 °C is studied. Due to the negative lattice mismatch of Ni-base superalloys, the N-type rafting with the formation of plate-like γ′precipitates occurs under uniaxial tensile loads along {100} direction at high temperatures, while the P-type rafting with the formation of rod-like γ′ precipitates occurs under compressive loads. Taking the cuboidal, N-type rafted and P-type rafted microstructures as the initial and fixed microstructures for the same loading conditions, it is found from DDD simulations that the rafted microstructures result in smaller creep deformation than the cuboidal microstructure. The reason for this is that the coalescence of γ′ precipitates during the rafting diminishes the width of some γ channels, so as to increase the local Orowan stresses which retard the dislocation glide. For tensile loads, the N-type rafted microstructure has the best creep resistance. For a low com- pressive load, the P-type rafting shows a better creep resistance than N-type rafting.

Temperature-independent giant dielectric response in transitional $BaTiO_3$ thin films

A. S. Everhardt, T. Denneulin, A. Grünebohm, Y.-T. Shao, P. Ondrejkovic, S. Zhou, N. Domingo, G. Catalan, J. Hlinka, J.-M. Zuo, S. Matzen, B. Noheda

Applied Physics Reviews, **7**, 11402 (2020)

Ferroelectric materials exhibit the largest dielectric permittivities and piezoelectric responses in nature, making them invaluable in applications from supercapacitors or sensors to actuators or electromechanical transducers. The origin of this behavior is their proximity to phase transitions. However, the largest possible responses are most often not utilized due to the impracticality of using temperature as a control parameter and to operate at phase transitions. This has motivated the design of solid solutions with morphotropic phase boundaries between different polar phases that are tuned by composition and that are weakly dependent on temperature. Thus far, the best piezoelectrics have been achieved in materials with intermediate (bridging or adaptive) phases. But so far, complex chemistry or an intricate microstructure has been required to achieve temperature-independent phase-transition boundaries. Here, we report such a temperature-independent bridging state in thin films of chemically simple $BaTiO_3$. A coexistence among tetragonal, orthorhombic, and their bridging low-symmetry phases are shown to induce continuous vertical polarization rotation, which recreates a smear in-transition state and leads to a giant temperature-independent dielectric response. The current material contains a ferroelectric state that is distinct from those at morphotropic phase boundaries and cannot be considered as ferroelectric crystals. We believe that other materials can be engineered in a similar way to contain a ferroelectric state with gradual change of structure, forming a class of transitional ferroelectrics. Similar mechanisms could be utilized in other materials to design low-power ferroelectrics, piezoelectrics, dielectrics, or shape-memory alloys, as well as efficient electro- and magnetocalorics.



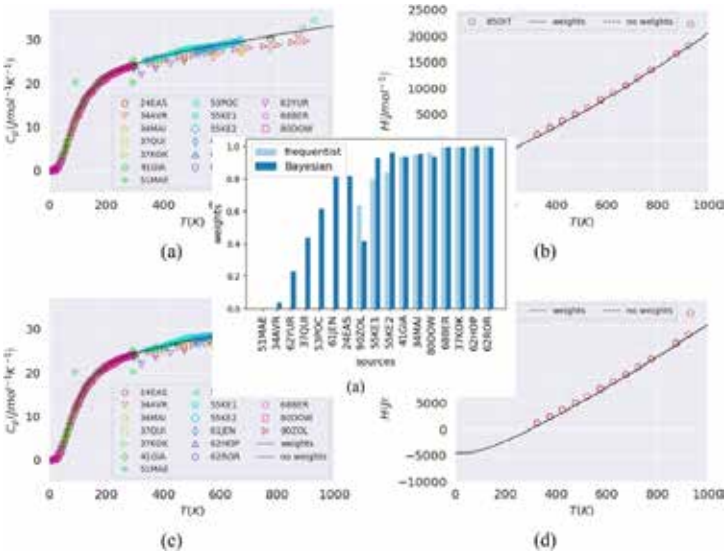
Transitional states with polarization rotation in chemical simple $BaTiO_3$ by strain engineering.

Comparison of statistically-based methods for automated weighting of experimental data in CALPHAD-type assessment

N. H. Paulson, S. Zomorodpoosh, I. Roslyakova, M. Stan

CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry, **68**, 101728 (2020)

The selection and weighting of experimental and simulated datasets is a necessary step in the development of thermodynamic property models in the calculation of phase diagrams (CALPHAD) approach. Currently, this step requires painstaking and complicated evaluation of the reliability of datasets and thermodynamic consistency between them. In this work, we present two novel and independently developed statistical approaches to aid in this process by addressing outliers and performing automated dataset weighting. The first method, presented here for the first time, applies classical statistical techniques and commonly available optimization algorithms. The second method employs Bayesian statistics via numerical sampling techniques. We compare the strengths and weaknesses of the two approaches through an assessment of the specific heat of aluminum and hafnium metal versus temperature for several experimental datasets. We then compare the weightings of each dataset versus a number of metrics employed by experts to evaluate the reliability of datasets.



Application of statistically-based methods for automated weighting of experimental data for pure Al in CALPHAD-type assessment.

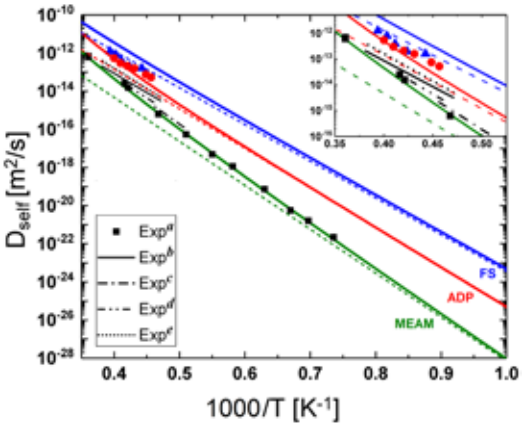
Atomistic description of self-diffusion in molybdenum: a comparative theoretical study of non-Arrhenius behavior

D. Smirnova, S. Starikov, G. Díaz Leines, Y. Liang, N. Wang, M. Popov, I. Abrikosov, D. G. Sangiovanni, R. Drautz, M. Mrovec

Physical Review Materials, **4**, 13605 (2020)

According to experimental observations, the temperature dependence of self-diffusion coefficient in most body-centered cubic metals (bcc) exhibits non-Arrhenius behavior. The origin of this behavior is likely related to anharmonic vibrational effects at elevated temperatures. However, it is still debated whether anharmonicity affects more the formation or migration of monovacancies, which are known to govern the self-diffusion. In this extensive atomistic simulation study we investigated thermodynamic properties of monovacancies in bcc molybdenum, here taken as a representative model system, from zero temperature to the melting point. We combined first-principles calculations and classical simulations based on three widely used interatomic potentials for Mo. In our analysis we employ static and dynamic atomistic calculations as well as statistical sampling techniques and thermodynamic integration to achieve thorough information about temperature variations of vacancy formation and migration free energies and diffusivities. In addition, we carry out large-scale molecular dynamics simulations that enable direct observation of high-temperature self-diffusion at the atomic scale. By scrutinizing the results obtained by different models and methods, we conclude that the peculiar self-diffusion behavior is likely caused by strong temperature dependence of the vacancy formation energy.

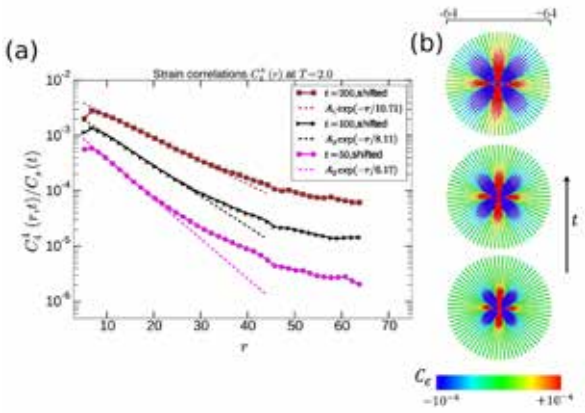
Comparison of theoretical and experimental temperature dependencies of self-diffusion coefficients for bcc Mo.



A crossover in spatio-temporal correlations of strain fluctuations in glass forming liquids

M. R. Hassani, M. Bruns, F. Varnik

Journal of Statistical Mechanics: Theory and Experiment (JSTAT), **2020**, 14002 (2020)



Via molecular dynamics simulations of a generic glass former in the supercooled and normal liquid states, it is shown that spatial correlations of strain fluctuations exhibit a crossover from the well-established power-law ~$1/r^3$-decay at long wavelengths to an exponential behavior, ~exp(-r/l_c) at intermediate distances. The characteristic length of the exponential decay grows both with temperature and time via l_c ~D(T)t, with D(T) being the temperature-dependent diffusion coefficient. This suggests that the crossover between the power-law and exponential decays is governed by a diffusion process.

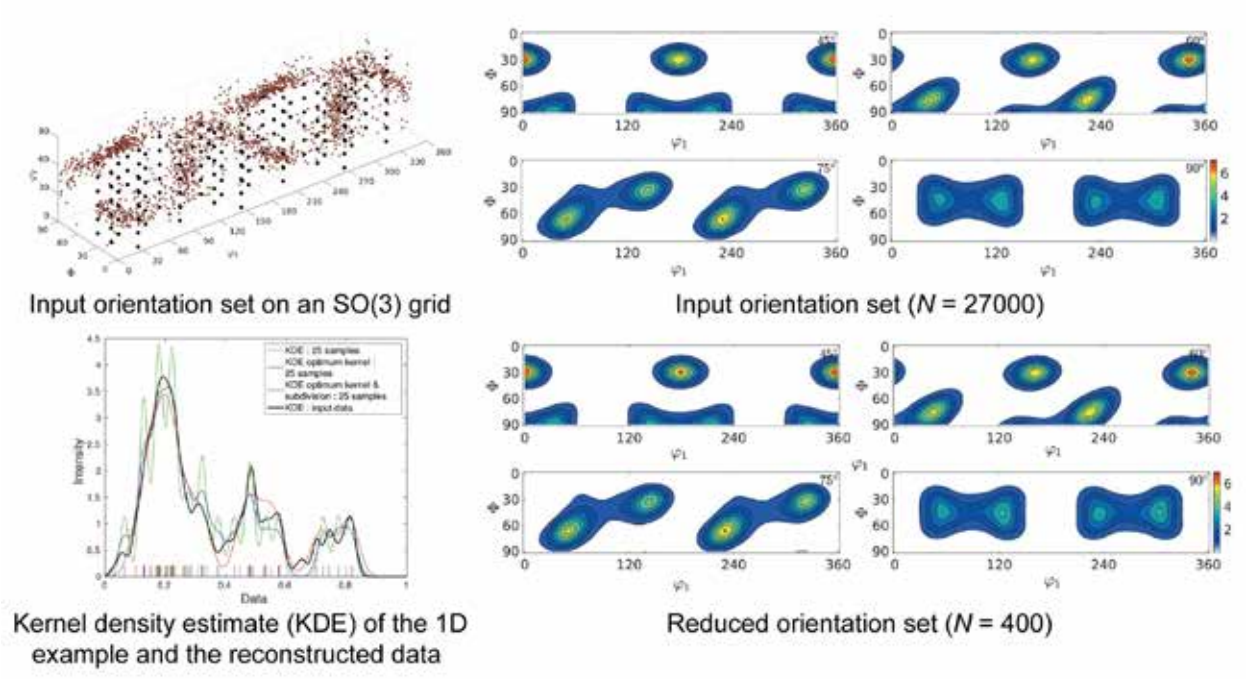
Left panel: The spatio-temporal correlations of strain fluctuations, $C_4^4(r, t)$, plotted in a semi-logarithmic scale at temperature of T= 2.0 (LJ unit; T_g=0.4), evaluated for three time intervals of t=50, 100, and 200 (LJ unit). The correlations in all three time intervals depict an initial exponential decay. The size of the exponential region expands by time which could reach up to 40 particle diameters for the case of t=200 (LJ unit). Right panel: 2D spatial evolution of the correlations are shown. Even though the exponential decay extends up to 40 particle diameters, the four-fold pattern of the correlations is preserved.

Optimized reconstruction of the crystallographic orientation density function based on a reduced set of orientations

A. Biswas, N. Vajragupta, R. Hielscher, A. Hartmaier
Journal of Applied Crystallography, **53**, 178-187 (2020)

Crystallographic textures, as they develop for example during cold forming, can have a significant influence on the mechanical properties of metals, such as plastic anisotropy. Textures are typically characterized by a non-uniform distribution of crystallographic orientations that can be measured by diffraction experiments like electron backscatter diffraction (EBSD). Such experimental data usually contain a large number of data points, which must be significantly reduced to be used for numerical modeling. However, the challenge in such data reduction is to preserve the important characteristics of the experimental data,while reducing the volume and preserving the computational efficiency of the numerical model. For example, in micromechanical modeling, representative volume elements (RVEs) of the real microstructure are generated and the mechanical properties of these RVEs are studied by the crystal plasticity finite element method. In this work, a new method is developed for extracting a reduced set of orientations from EBSD data containing a large number of orientations. This approach is based on the established integer approximation method and it minimizes its shortcomings. Furthermore, theL1norm is applied as an error function; this is commonly used in texture analysis for quantitative assessment of the degree of approximation and can be used to control the convergence behavior. The method is tested on four experimental data sets to demonstrate its capabilities. This new method for the purposeful reduction of a set of orientations into equally weighted orientations is not only suitable for numerical simulation but also shows improvement in results in comparison with other available methods.

Reconstruction of the orientation distribution function of polycrystalline materials, and application using CPFEM.

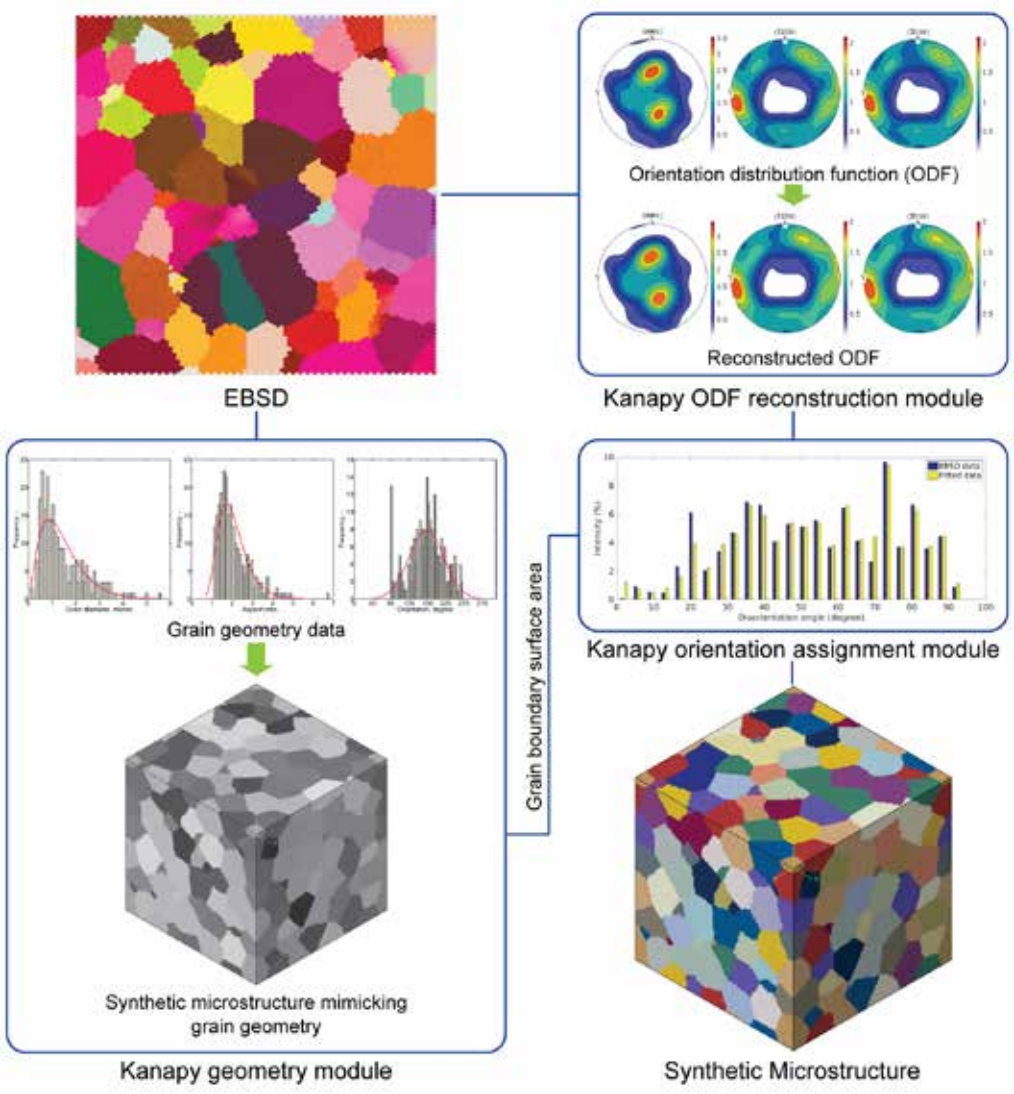


Kanapy:
Synthetic polycrystalline microstructure generator with geometry and texture

A. Biswas, M. Ramaswamy Guru Prasad, N. Vajragupta, A. Hartmaier
Zenodo Repository (2020)

In Kanapy-v1, an efficient modeling strategy for generating the geometry of the synthetic microstructures using statistical data was presented. Some of the novel features provided include: modeling complex microstructures consisting of irregular grain shapes, particle (grain) packing through collision detection and response system, and collision handling through a two-layer collision detection scheme. Synthetic microstructures are a key aspect of the micromechanical modeling approach for the prediction of mechanical properties. Apart from microstructure geometry, a vital component of polycrystalline microstructures that has substantial influence on the material behavior is texture. Therefore, a synthetic microstructure can be considered incomplete without the information of texture. This is addressed in the current version of Kanapy by including new efficient texture reduction and orientation assignment algorithms to the already existing package.

Version 2 of the previously developed synthetic microstructure generator KANAPY, including the texture module for orientation and disorientation reconstruction.

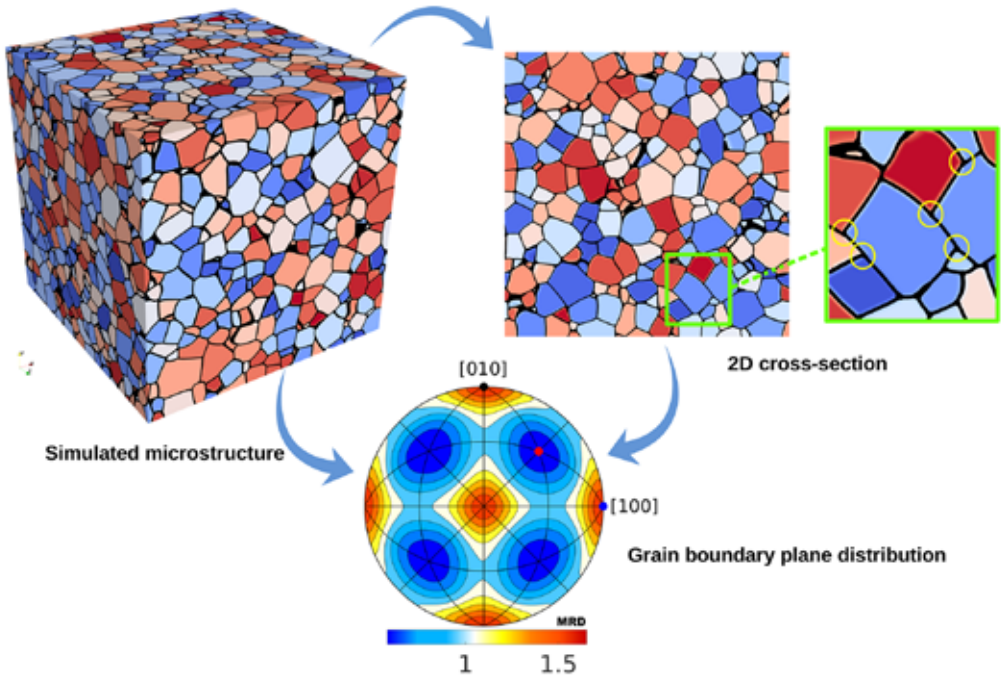


Role of inclination dependence of grain boundary energy on the microstructure evolution during grain growth

H. F. Salama, J. Kundin, O. Shchyglo, V. Mohles, K. Marquardt, I. Steinbach

Acta Materialia, **188**, 641-651 (2020)

The role of inclination dependence of grain boundary energy on the microstructure evolution and the orientation distribution of grain boundary planes during grain growth in polycrystalline materials is investigated by three-dimensional phase-field simulations. The anisotropic grain boundary energy model uses the description of the faceted surface structure of the individual crystals and constructs an anisotropic energy of solid-solid interface. The energy minimization occurs by the faceting of the grain boundary due to inclination dependence of the grain boundary energy. The simulation results for a single grain show the development of equilibrium shapes (faceted grain morphologies) with different families of facets which agrees well with the theoretical predictions. The results of grain growth simulations with isotropic and anisotropic grain boundary energy for cubic symmetry show that inclination dependence of grain boundary energy has a significant influence on the grain boundary migration, grain growth kinetics and the grain boundary plane distribution. It has been shown that the model essentially reproduces the experimental studies reported for NaCl and MgO polycrystalline systems where the anisotropic distribution of grain boundary planes has a peak for the low-index {100} type boundaries.

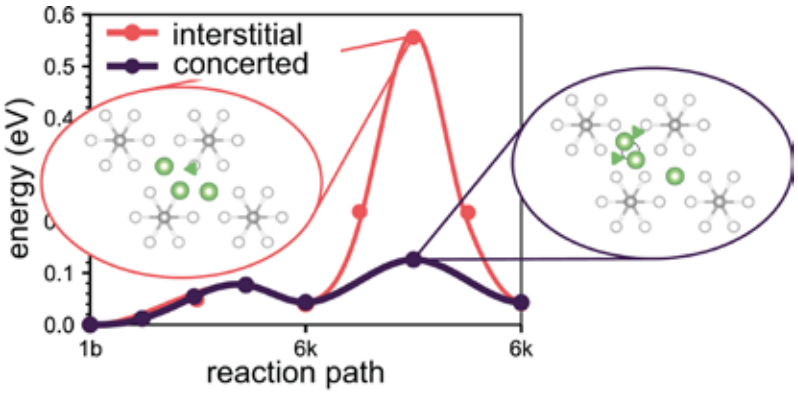


Three-dimensional evolved microstructure under the effect of anisotropic grain boundary energy (top left). A cross-section of the simulated microstructure indicates the presence of more cubic grains with triple-junction angles close to 90 and 180 degrees (top right). The grain boundary plane distribution has a peak for the low-index {100} type boundaries (down).

Fast diffusion mechanism in $Li_4P_2S_6$ via a concerted process of interstitial Li ions

A. Stamminger, B. Ziebarth, M. Mrovec, T. Hammerschmidt, R. Drautz
RSC Advances, **10**, 10715-10722 (2020)

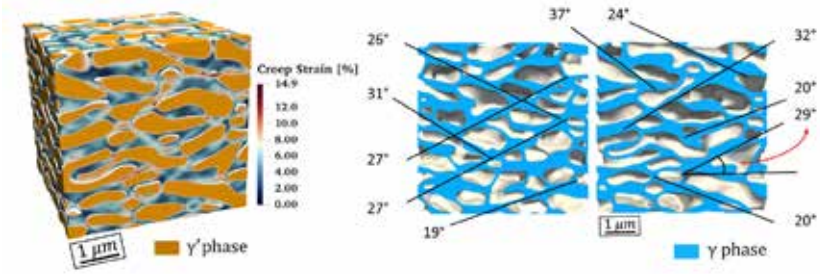
The synthesis of Li superionic conductor $Li_7P_3S_{11}$ may be accompanied by the formation of a detrimental $Li_4P_2S_6$ phase due to a high mixing sensitivity of precursor materials. This phase exhibits a poor ionic conductivity whose origins are not fully understood. Recently Dietrichet al.investigated the energetics of Li ion migration in $Li_4P_2S_6$ with nudged elastic band (NEB) calculations. The observed large migration barrier of 0.51 e.V. for purely interstitial diffusion leads to an interpretation of the low ionic conductivity by kinetic limitations. Based on ab initio molecular dynamics simulations (AIMD) we propose a new and energetically much more favorable diffusion path available to interstitial Li ion charge carriers that has not been considered so far. It consists of a concerted process in which a second lithium atom is pushed out from its equilibrium lattice position by the diffusing lithium ion. A detailed analysis with NEB calculations shows that the energy barrier for this concerted diffusion is only 0.08 eV, i.e. an order of magnitude lower than the previously reported value for purely interstitial diffusion. Therefore, the observed low ionic conductivity of $Li_4P_2S_6$ is likely not originating from kinetic limitations due to high diffusion barriers but rather from thermodynamic reasons associated with a low concentration of free charge carriers. We therefore expect that increasing the charge carrier concentration by doping is a viable design route to optimize the ionic conductivity of this material.



Fast diffusion mechanism in $Li_4P_2S_6$ via a concerted process of interstitial Li ions identified by ab-initio calculations.

45-degree rafting in Ni-based superalloys: A combined phase-field and strain gradient crystal plasticity study

M. A. Ali, W. Amin, O. Shchyglo, I. Steinbach
International Journal of Plasticity, **128**, 102659 (2020)



Phase field-crystal plasticity simulation of 45° rafting in a Ni-based single crystal superalloy.

45° rafting of Ni-based superalloys has been investigated with the help of creep test simulations applying a strain gradient crystal plasticity model coupled to the multi-phase field method. This mode of rafting lies in between P- and N-type rafting modes. The model parameters are calibrated against experimental data for N-type rafting under high temperature and low stress creep condition. By increasing the stress level, the mixed-mode rafting of precipitates with a clear tendency toward formation of 45° rafts is observed. We show that the key factor for the occurrence of this type of rafting is the generation of highly localized creep strain of more than 10 % due to non-homogeneous creep deformation in the form of slip bands. We have successfully captured the evolution of microstructure under high stress leading to production of localized shear bands.

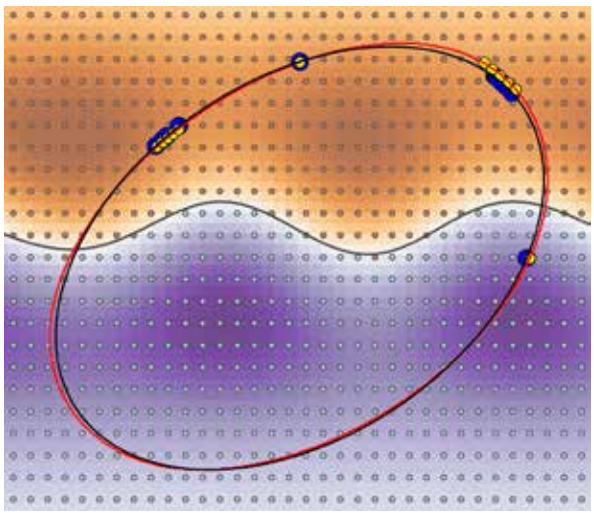
Data-oriented constitutive modeling of plasticity in metals

A. Hartmaier

Materials, **13**,1600 (2020)

Constitutive models for plastic deformation of metals are typically based on flow rules determining the transition from elastic to plastic response of a material as function of the applied mechanical load. These flow rules are commonly formulated as a yield function, based on the equivalent stress and the yield strength of the material, and its derivatives. In this work, a novel mathematical formulation is developed that allows the efficient use of machine learning algorithms describing the elastic-plastic deformation of a solid under arbitrary mechanical loads and that can replace the standard yield functions with more flexible algorithms. By exploiting basic physical principles of elastic-plastic deformation, the dimensionality of the problem is reduced without loss of generality. The data-oriented approach inherently offers a great flexibility to handle different kinds of material anisotropy without the need for explicitly calculating a large number of model parameters. The applicability of this formulation in finite element analysis is demonstrated, and the results are compared to formulations based on Hill-like anisotropic plasticity as reference model. In future applications, the machine learning algorithm can be trained by hybrid experimental and numerical data, as for example obtained from fundamental micromechanical simulations based on crystal plasticity models. In this way, data-oriented constitutive modeling will also provide a new way to homogenize numerical results in a scale-bridging approach.

Machine learning algorithm can be trained to capture plastic properties of metals.

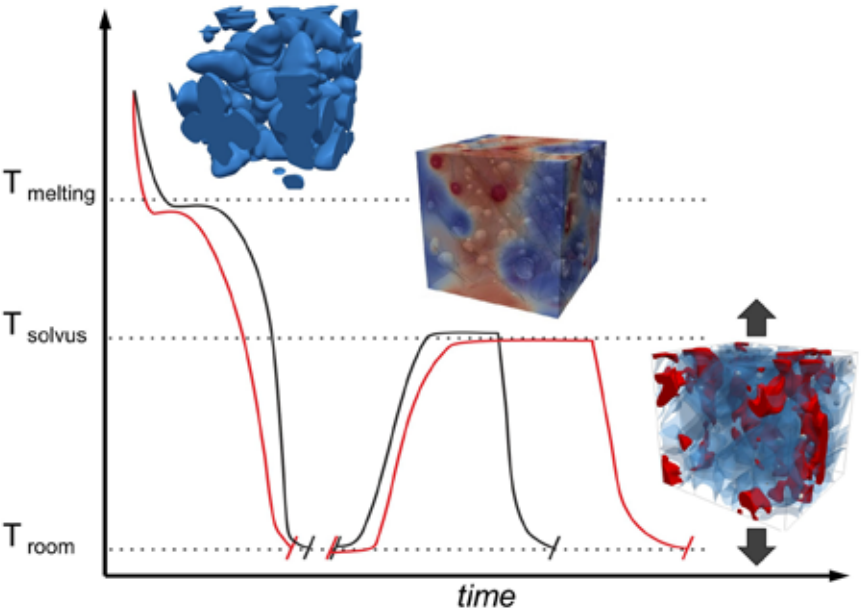


Roadmap on multiscale materials modeling

E. van der Giessen, P. A. Schultz, N. Bertin, V. V. Butalov, W. Cai, G. Csanyi, S. M. Foiles, M. G. D. Geers, C. Gonzales, M. Hütter, W. K. Kim, D. Kochmann, J. Llorca, A. E. Mattson, J. Rottler, A. Shluger, R. B. Sills, I. Steinbach, A. Strachan, E. B. Tadmor

Modelling and Simulation in Materials Science and Engineering, **28**, 43001 (2020)

Modeling and simulation is transforming modern materials science, becoming an important tool for the discovery of new materials and material phenomena, for gaining insight into the processes that govern materials behavior, and, increasingly, for quantitative predictions that can be used as part of a design tool in full partnership with experimental synthesis and characterization. Modeling and simulation is the essential bridge from good science to good engineering, spanning from fundamental understanding of materials behavior to deliberate design of new materials technologies leveraging new properties and processes. This Roadmap presents a broad overview of the extensive impact computational modeling has had in materials science in the past few decades, and offers focused perspectives on where the path forward lies as this rapidly expanding field evolves to meet the challenges of the next few decades. The Roadmap offers perspectives on advances within disciplines as diverse as phase field methods to model mesoscale behavior and molecular dynamics methods to deduce the fundamental atomic-scale dynamical processes governing materials response, to the challenges involved in the interdisciplinary research that tackles complex materials problems where the governing phenomena span different scales of materials behavior requiring multiscale approaches. The shift from understanding fundamental materials behavior to development of quantitative approaches to explain and predict experimental observations requires advances in the methods and practice in simulations for reproducibility and reliability, and interacting with a computational ecosystem that integrates new theory development, innovative applications, and an increasingly integrated software and computational infrastructure that takes advantage of the increasingly powerful computational methods and computing hardware.

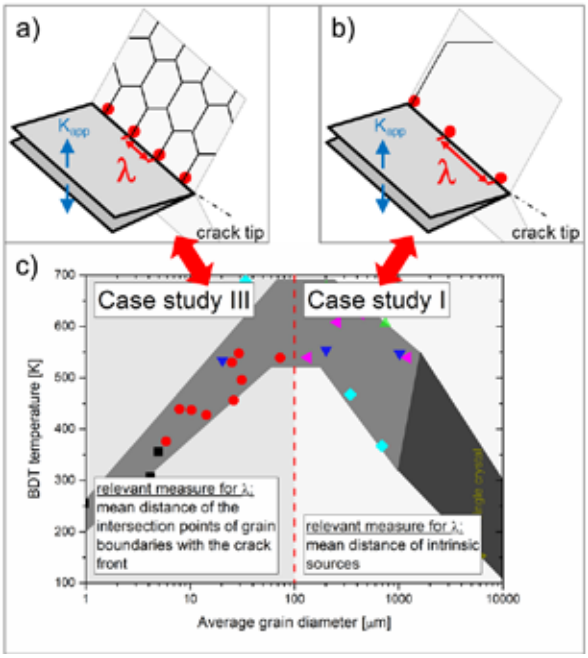


Scheme of two different production cycles (from solidification to failure). The microstructure will evolve during the whole life-time cycle of a material, dependent on temperature and various environmental loads. The microstructure memorizes the whole history of production and service, which determine the property of the material. The properties at the end of different cycles will be different!

Elucidating the dual role of grain boundaries as dislocation sources and obstacles and its impact on toughness and brittle-to-ductile transition

J. Reiser, A. Hartmaier
Scientific Reports, **10**, 2739 (2020)

In this paper, we resolve the role of grain boundaries on toughness and the brittle-to-ductile transition. On the one hand, grain boundaries are obstacles for dislocation glide. On the other hand, the intersection points of grain boundaries with the crack front are assumed to be preferred dislocation nucleation sites. Here, we will show that the single contributions of grain boundaries (obstacles vs. source) on toughness and the brittle-to-ductile transition are contradicting, and we will weight the single contributions by performing carefully designed numerical experiments by means of two-dimensional discrete dislocation dynamics modelling. In our parameter studies, we vary the following parameters: (i) the mean free path for dislocation glide, δ, combined with (ii) the (obstacle) force of the grain boundary, φ, and (iii) the dislocation source spacing along the crack front, λ. Our results show that for materials or microstructures for which the mean distance of the intersection points of grain boundaries with the crack front is the relevant measure for λ, a decrease of grain size results in an increase of toughness. The positive impact of grain boundaries outweighs the negative consequences of dislocation blocking. Furthermore, our results explain the evolving anisotropy of toughness in cold-worked metals and give further insight into the question of why the grain-size-dependent fracture toughness passes through a minimum (and the brittle-to-ductile transition temperature passes through a maximum) at an intermediate grain size. Finally, a relation of the grain-size-dependence of fracture toughness in the form of $K(d\delta, d\lambda) = KIC + kd\delta 0.5/d\lambda$ is deduced.



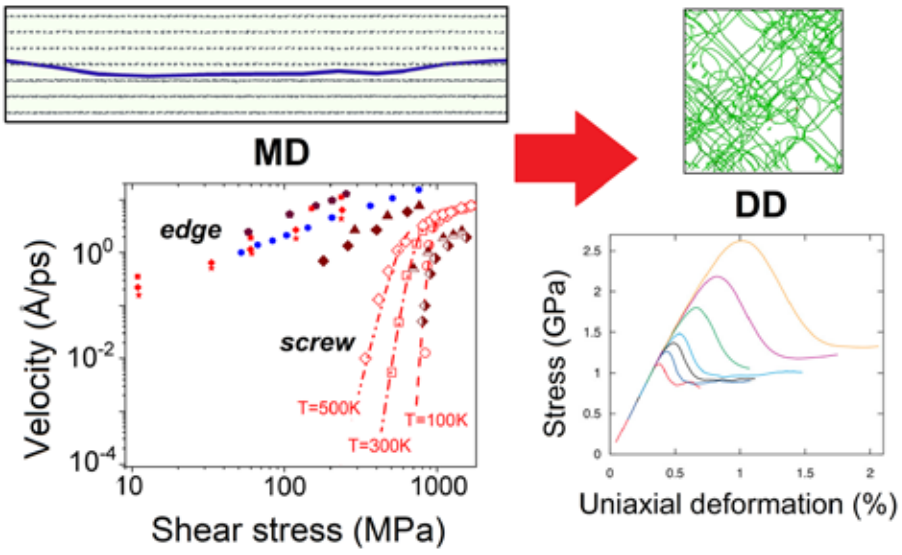
The BDT temperature passes through a maximum at an intermediate grain size. For materials or microstructures for which the intersection points of grain boundaries with the crack front is the relevant measure for λ, a decrease of grain size results in a decrease of the transition temperature (a). For microstructures for which the mean distance of intrinsic sources is the relevant measure for λ, a decrease of grain size results in an increase of the transition temperature (b). In (c), the data is discussed against the background of the mean findings of our numerical experiments.

Two-scale simulation of plasticity in molybdenum: combination of atomistic simulation and dislocation dynamics with non-linear mobility function

S. Starikov, V. Tseplyaev

Computational Materials Science, **179**, 109585 (2020)

We present multi-scale simulation of plastic deformation in molybdenum. The temperature-dependent mobility functions of screw and edge dislocations were calculated from molecular dynamics simulation with two different interatomic potentials. The simulations of screw dislocation movement under applied shear stress revealed that the process can proceed in two different regimes: through thermally activated motion and athermal motion. Hence, the dislocation velocity depends on the shear stress in a non-trivial way. We took this fact into account during calculation of the mobility functions and their implementation in the dislocation dynamics (DD) model. Such model allows us to simulate plastic deformation with consideration of temperature effect on the dislocation mobility. Here we discuss the changes in DD predictions depending on the input parameters obtained from the atomistic simulation. As the main result, we report the yield stress calculated for a single crystal of molybdenum at various temperatures, strain rates, and dislocation densities. Thoroughly discussed comparison of the simulation results with the available experimental data gives opportunity to estimate the accuracy of the created multi-scale model.



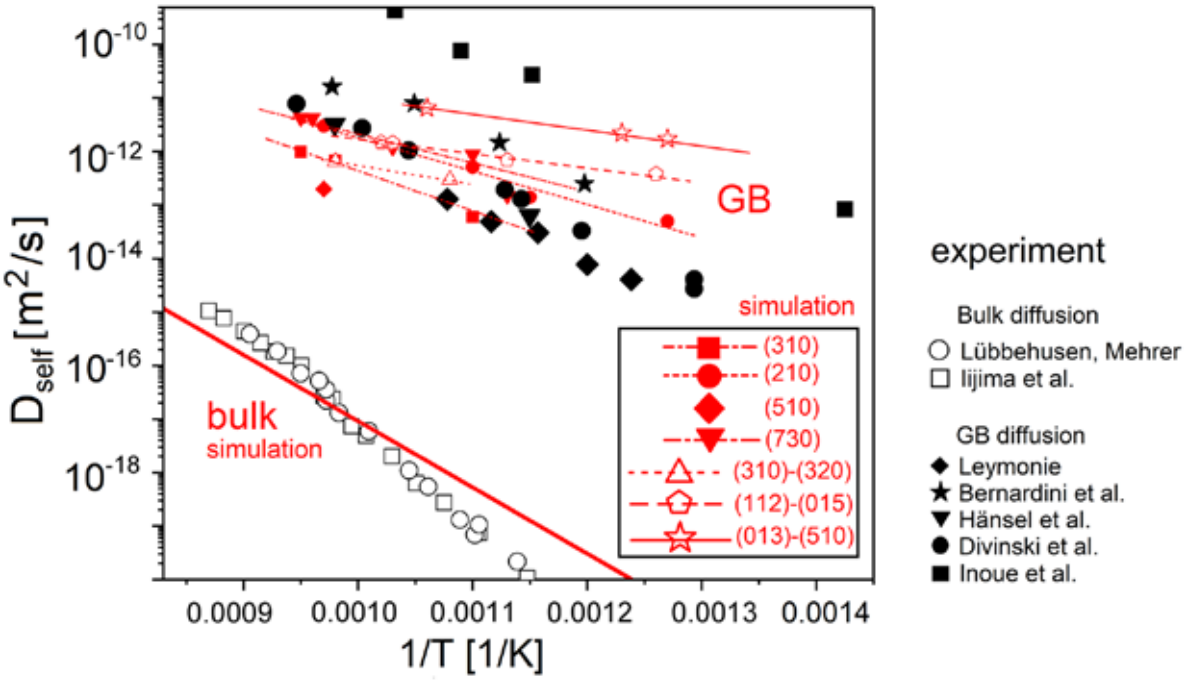
Two-scale simulation of plasticity in molybdenum: from molecular dynamics simulation of dislocation mobility to dislocation dynamics simulation of plastic deformation.

Study of grain boundary self-diffusion in iron with different atomistic models

S. Starikov, M. Mrovec, R. Drautz
Acta Materialia, **188**, 560-569 (2020)

We studied grain boundary (GB) self-diffusion in body-centered cubic iron using ab initio calculations and molecular dynamics simulations with various interatomic potentials. A combination of different models allowed us to determine the principal characteristics of self-diffusion along different types of GBs. In particular, we found that atomic self-diffusion in symmetric tilt GBs is mostly driven by self-interstitial atoms. In contrast, in general GBs atoms diffuse predominantly via an exchange mechanism that does not involve a particular defect but is similar to diffusion in a liquid. Most observed mechanisms lead to a significant enhancement of self-diffusion along GBs as compared to diffusion in the bulk. The results of simulations are verified by comparison with available experimental data.

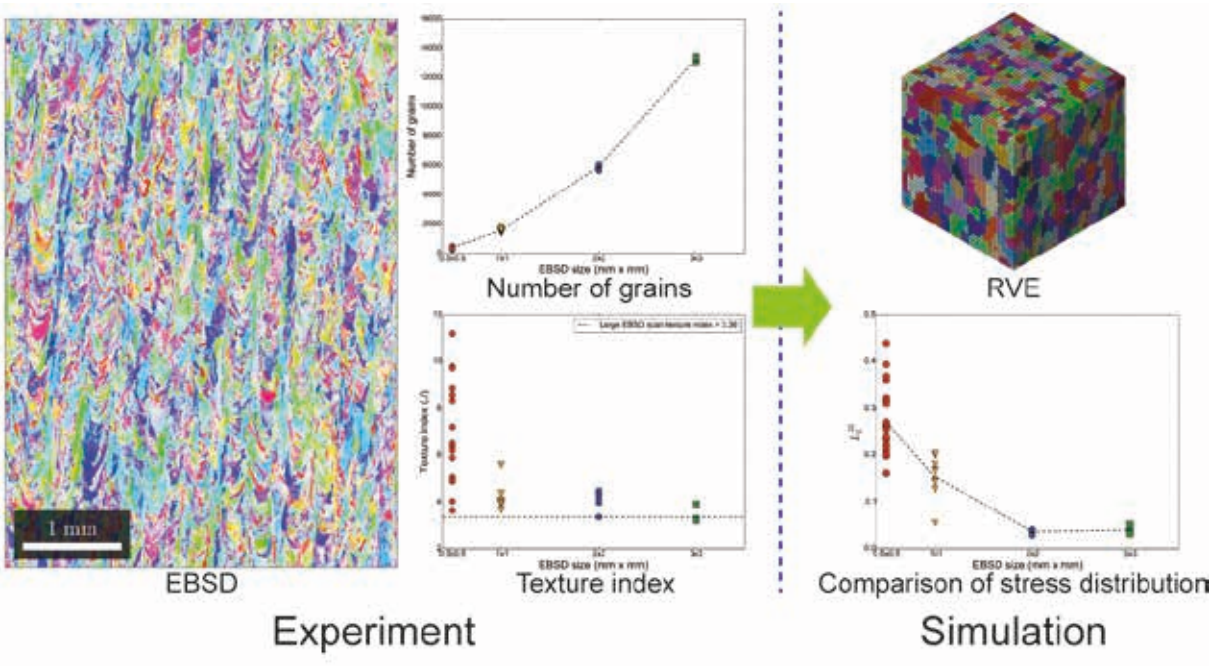
Calculated bulk and GB self-diffusion coefficients of iron in comparison with available experimental data.



Effect of grain statistics on micromechanical modeling: the example of additively manufactured materials examined by electron backscatter diffraction

A. Biswas, M. Ramaswamy Guru Prasad, N. Vajragupta, A. Kostka, T. Niendorf, A. Hartmaier
Advanced Engineering Materials, **22**, 1901416 (2020)

Micromechanical modeling is one of the prominent numerical tools for the prediction of mechanical properties and the understanding of deformation mechanisms of metals. As input parameters, it uses data obtained from microstructure characterization techniques, among which the electron backscatter diffraction (EBSD) technique allows us to understand the nature of microstructural features, that are usually described by statistics. Because of these advantages, the EBSD dataset is widely used for synthetic microstructure generation. However, for the statistical description of microstructural features, the population of input data must be considered. Preferably, the EBSD measurement area must be sufficiently large to cover an adequate number of grains. However, a comprehensive study of this measurement area with a crystal plasticity finite element method (CPFEM) framework is still missing although it would considerably facilitate information exchange between experimentalists and simulation experts. Herein, the influence of the EBSD measurement area and the number of grains on the statistical description of the microstructural features and studying the corresponding micromechanical simulation results for 316L stainless steel samples produced by selective laser melting is investigated.

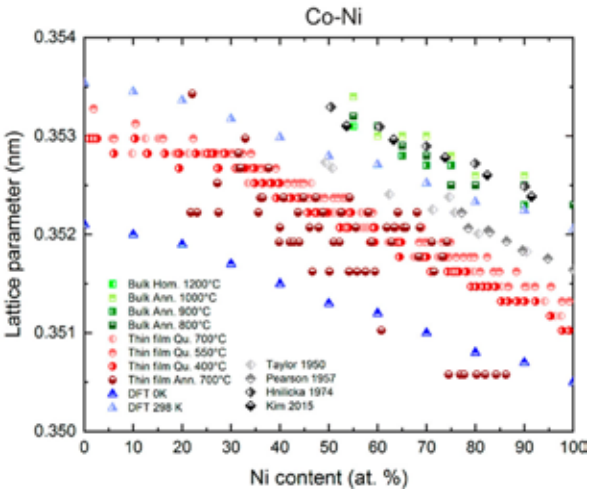


Optimum EBSD size for reliable micromechancial modeling.

Experimental and theoretical investigation on phase formation and mechanical properties in Cr–Co–Ni alloys processed using a novel thin-film quenching technique

D. Naujoks, M. Schneider, S. Salomon, J. Pfetzing-Micklich, A. P. Subramanyam, T. Hammerschmidt, R. Drautz, J. Frenzel, A. Kostka, G. Eggeler, G. Laplanche, A. Ludwig
ACS Combinatorial Science, **22**, 232-247 (2020)

The Cr-Co-Ni system was studied by combining experimental and computational methods to investigate phase stability and mechanical properties. Thin-film materials libraries were prepared and quenched from high temperatures up to 700°C using a novel quenching technique. It could be shown that a wide A1 solid solution region exists in the Cr-Co-Ni system. To validate the results obtained using thin-film materials libraries, bulk samples of selected compositions were prepared by arc melting, and the experimental data were additionally compared to results from DFT calculations. The computational results are in good agreement with the measured lattice parameters and elastic moduli. The lattice parameters increase with the addition of Co and Cr, with a more pronounced effect for the latter. The addition of ~20 atom % Cr results in a similar hardening effect to that of the addition of ~40 atom % Co.

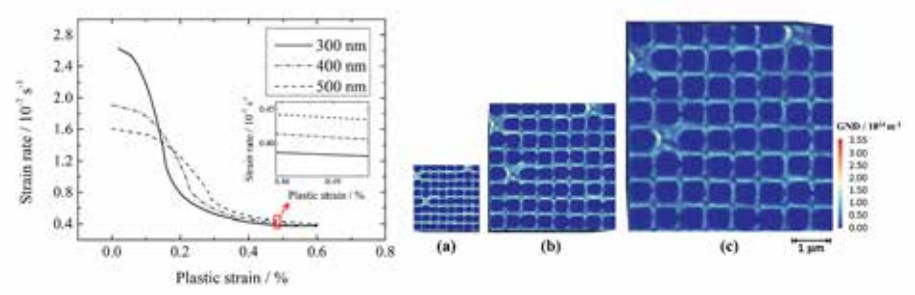


Composition dependence of lattice parameter of Co-Ni solid-solution phase as obtained from bulk samples, thin-film samples and ab-initio calculations.

Effect of γ′ precipitate size on hardness and creep properties of Ni-base single crystal superalloys: experiment and simulation

M. A. Ali, I. Lopez-Galilea, W. Amin, S. Gao, O. Shchyglo, A. Hartmaier, W. Theisen, I. Steinbach
Materialia, **12**, 100692 (2020)

The role and effect of γ′ precipitate size on the mechanical properties of Ni-base single crystal superalloy is investigated. The underlying mechanisms are analyzed on the one hand with the help of experiments including hardness and creep tests, and on the other hand with the help of two different simulation approaches by taking the typical γ/γ′ microstructure into account. Simulations, based on the crystal plasticity finite element method (CPFEM) are carried out for the hardness tests, whereas simulations, based on the crystal plasticity coupled phase-field method (CPPFM) are carried out for the creep tests. The hardness test simulation results show that the hardness of material varies inversely with the size of γ′ precipitates for a given γ′phase volume fraction and it varies directly with the volume fraction of γ′ precipitates for a given precipitate size. These results are qualitatively consistent with the experimental observations. The creep simulation results show that the refinement of γ′ precipitates with a certain volume fraction of precipitates leads to an improvement of creep resistance by delaying the plastic activity in the material.



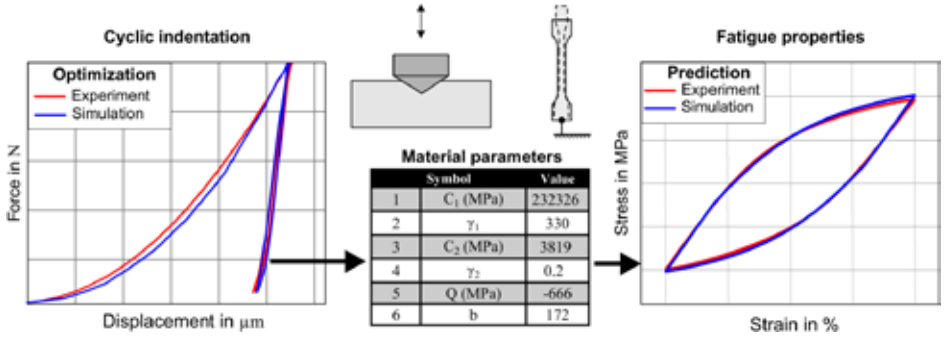
Evolution of plastic strain rate for different γ′ precipitate sizes (left). GND are displayed in the γ channels for different γ′ sizes: (a) 300 nm, (b) 400 nm and (c) 500 nm (right).

Inverse method to determine fatigue properties of materials by combining cyclic indentation and numerical simulation

H. Sajjad, H. u. Hassan, M. Kuntz, B. J. Schaefer, P. Sonnweber-Ribic, A. Hartmaier

Materials, Special Issue Recent Advances in Mechanisms of Fracture and Fatigue, **13**, 3126 (2020)

The application of instrumented indentation to assess material properties like Young's modulus and microhardness has become a standard method. In recent developments, indentation experiments and simulations have been combined to inverse methods, from which further material parameters such as yield strength, work hardening rate, and tensile strength can be determined. In this work, an inverse method is introduced by which material parameters for cyclic plasticity, i.e., kinematic hardening parameters, can be determined. To accomplish this, cyclic Vickers indentation experiments are combined with finite element simulations of the indentation with unknown material properties, which are then determined by inverse analysis. To validate the proposed method, these parameters are subsequently applied to predict the uniaxial stress–strain response of a material with success. The method has been validated successfully for a quenched and tempered martensitic steel and for technically pure copper, where an excellent agreement between measured and predicted cyclic stress–strain curves has been achieved. Hence, the proposed inverse method based on cyclic nanoindentation, as a quasi-nondestructive method, could complement or even substitute the resource-intensive conventional fatigue testing in the future for some applications.



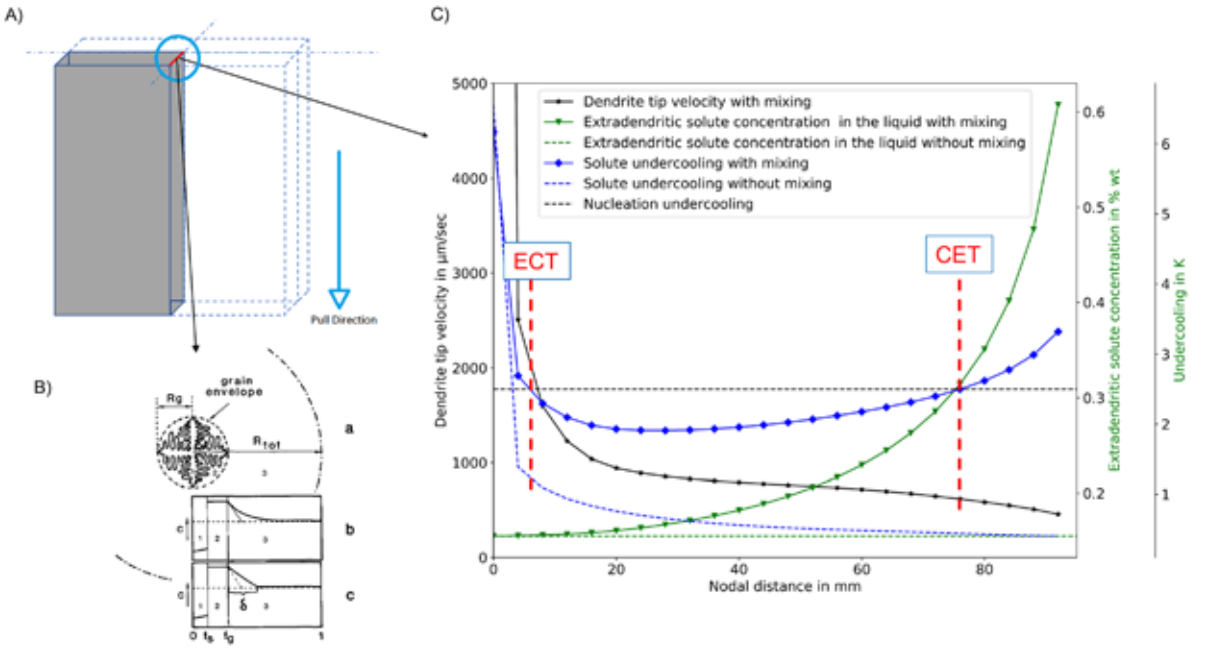
Predicting fatigue properties from cyclic indentation.

Columnar-equiaxed transition in continuous casting based on a micromacro solidification model with long-range solutal mixing

M. Uddagiri, S. Hubig, J. Spee, I. Steinbach

IOP conference series: Materials science and engineering, **861**, 12014 (2020)

A novel model is proposed to describe the columnar to equiaxed transition (CET) in continuous casting. The model bases on Rappaz and Thevoz's solute diffusion model for equiaxed dendritic growth, combined with a 1-Dimensional solidification model normal to the slab surface. The unique feature of the proposed model is the combination with a mixing term between interdendritic and extradendritic melt, representing long-range solutal mixing by convection. The model can also be applied to predict equiaxed to columnar transition (ECT), i.e. the chill zone thickness. The model consists of modules such as nucleation, growth kinetics, solute and heat balance, and a solute mixing module. Nucleation is considered with a fixed nucleation undercooling. The growth kinetics of the dendrites are treated according to the LGK model. A finite difference scheme is employed for solving 1-Dimensional heat transfer equations and finally, volume averaged solute balance equations are solved in a staggered scheme. Mixing of inter- and extradendritic liquid is, as a first step, treated ideally fast. When applied to Fe-C binary system with the thermo-physical properties obtained from literature and CALPHAD simulations, the model successfully predicts recalescence, phase fraction evolution, and concentration profiles in different phases. Realistic boundary conditions of the continuous casting process are obtained from macroscopic FEM simulation.

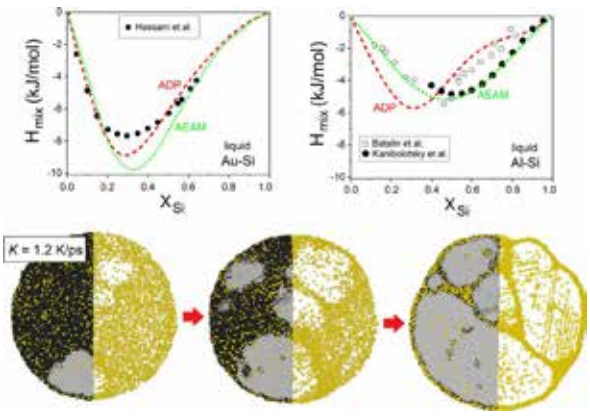


A) schematic representation of a quarter of a steel slab produced by continuous casting process. 1D system of control volumes are highlighted with a red line. B) Schematic representation of Rappaz Thevoz model used to model the solidification phenomena C) Results obtained for solute undercooling, dendrite tip velocity and solute enrichment when simulated with (solid lines) and without (dotted lines) macroscopic solute mixing. Equiaxed Columnar Transition (ECT or Chill zone) and Columnar Equiaxed Transition (CET) can be identified by comparing solute undercooling and nucleation undercooling.

Optimized interatomic potential for study of structure and phase transitions in Si-Au and Si-Al systems

S. Starikov, I. Gordeev, Y. Lysogorskiy, L. Kolotova, S. Makarov
Computational Materials Science, **184**,109891 (2020)

Metal-semiconductor nanostructures are key objects for multifunctional electronics and optical design. We report a new interatomic potential for atomistic simulation of a ternary Si-Au-Al system. The development procedure was based on the force-matching method that allowed us to create the potential without use of experimental data at the fitting. Extensive validation including elastic, thermophysical and defect properties demonstrates a wide range of the potential applicability. Special attention was paid to the description of the silicon-metal alloys in liquid and amorphous states. We used the new potential for study of crystallization and glass transition in the undercooled melt. The simulation results revealed the beneficial conditions for the formation of the unique metal-semiconductor nanocrystalline structure, which is highly important for various applications in the field of nanophotonics.

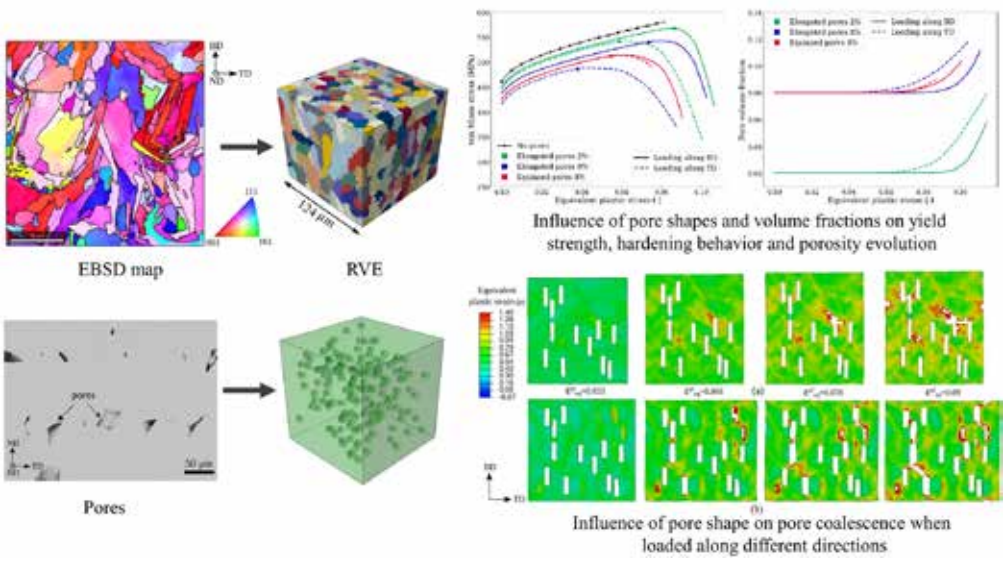


(upper panel) Mixing energy for Au-Si and Al-Si alloys; (lower panel) atomistic simulation of crystallization in Au-Si alloy.

Influence of pore characteristics on anisotropic mechanical behavior of L-PBF manufactured metal by micromechanical modeling

M. Ramaswamy Guru Prasad, A. Biswas, W. Amin, S. Gao, K. Geenen, J. Lian, A. Röttger, N. Vajragupta, A. Hartmaier
Advanced Engineering Materials, 2000641 (2020)

In recent times, Additive Manufacturing (AM) has proven to be an indispensable technique for processing complex three-dimensional parts because of the versatility and ease of fabrication it offers. However, the generated microstructures show a high degree of complexity due to the complex solidification process of the melt pool. In this study, micromechanical modeling is applied to gain deeper insight into the influence of defects on plasticity and damage of 316L stainless steel specimens produced by laser powder bed fusion (L-PBF) process. With the statistical data obtained from microstructure characterization, the complex AM microstructures are modeled by a synthetic microstructure generation tool. A damage model in combination with an element deletion technique is implemented into a non-local crystal plasticity model, to describe anisotropic mechanical behaviour including damage evolution. The element deletion technique is applied to effectively model the growth and coalescence of microstructural pores as described by a damage parameter. Numerical simulations show that the shape of the pores not only affects the yielding and hardening behavior but also influences the porosity evolution itself.

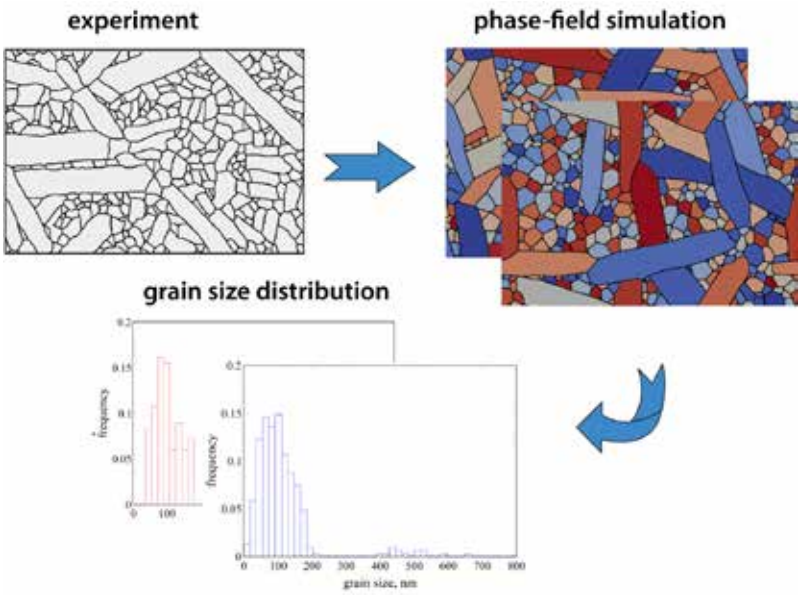


Micromechanical modeling scheme to assess the influence of pore characteristics on anisotropic mechanical behavior of additively manufactured metal.

Phase-field simulation of abnormal anisotropic grain growth in polycrystalline ceramic fibers

J. Kundin, R. S. M. Almeida, H. F. Salama, H. Farhandi, K. Tushtev, K. Rezwan
Computational Materials Science, **185**, 109926 (2020)

The present work proposes a phase-field approach to realistically simulate abnormal grain growth in polycrystalline ceramic fibers at temperatures above 1000 °C. Under these conditions, grain growth is characterized by the formation of large elongated rectangular grains in a matrix of normal grains. The multi-phase-field model is extended by mechanisms which are responsible for the abnormal anisotropic growth: anisotropic interface energy, anisotropic interface mobility and a recrystallization driving force. Two types of mobility anisotropy are considered: anisotropy due to the misorientation between grains and anisotropy due to the dependency on inclination angles. The experimental data from heat treatments of the ceramic fiber Nextel 610 at 1200–1300 °C with different dwell times are examined by the proposed model. The comparison of the experiment and the simulation results at various times shows that the extended multi-phase-field model is able to simulate the microstructure realistically. In most model cases, abnormal grains have a rectangular shape, similar to the experiment. The best fit of the experimental grain size distribution and the grain shape is achieved by the simulation with the misorientation dependency of the interface mobility. Furthermore, it was shown that a strong decrease on the grain growth rate with time, observed in the experiment, can be reproduced by the simulations taking into account the segregation of impurities on grain boundaries that results in the decreasing grain boundary mobility.

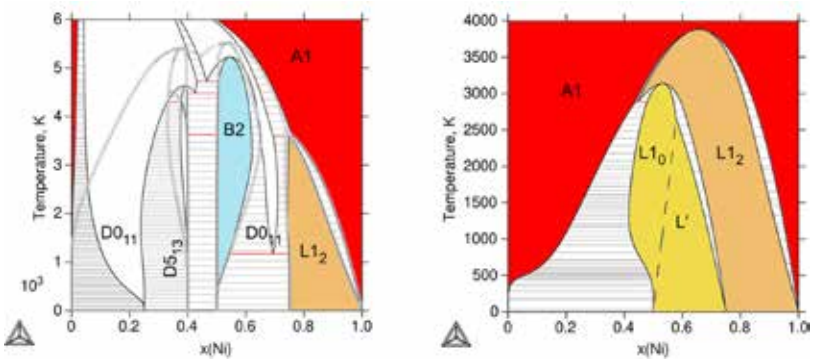


Experimental microstructure as used in digital image analysis (top left), simulated microstructure with anisotropic abnormal grains for various heat treatment temperatures and time (top right) and comparison of the experimental and simulated grain size distribution (bottom).

DFT-CEF approach for the thermodynamic properties and volume of stable and metastable Al–Ni compounds

S. D. Tumminello, M. Palumbo, J. Koßmann, T. Hammerschmidt, P. R. Alonso, S. Sommadossi, S. G. Fries
Metals, **10**, 1142 (2020)

The Al–Ni system has been intensively studied both experimentally and theoretically. Previous first-principles calculations based on density-functional theory (DFT) typically investigate the stable phases of this system in their experimental stoichiometry. In this work, we present DFT calculations for the Al–Ni system that cover stable and metastable phases across the whole composition range for each phase. The considered metastable phases are relevant for applications as they are observed in engineering alloys based on Al–Ni. To model the Gibbs energies of solid phases of the Al–Ni system, we combine our DFT calculations with the compound energy formalism (CEF) that takes the Bragg–Williams–Gorsky approximation for the configurational entropy. Our results indicate that the majority of the investigated configurations have negative energy of formation with respect to Al fcc and Ni fcc. The calculated molar volumes for all investigated phases show negative deviations from Zen's law. The thermodynamic properties at finite temperatures of individual phases allow one to predict the configurational contributions to the Gibbs energy. By applying a fully predictive approach without excess parameters, an acceptable topology of the DFT-based equilibrium phase diagram is obtained at low and intermediate temperatures. Further contributions can be added to improve the predictability of the method, such as phonons or going beyond the Bragg–Williams–Gorsky approximation that overestimates the stability range of the ordered phases. This is clearly demonstrated in the fcc order/disorder predicted metastable phase diagram.



Phase diagrams of stable (left) and metastable (right) phases in the Al-Ni system computed with the compound-energy formalism and density-functional theory.

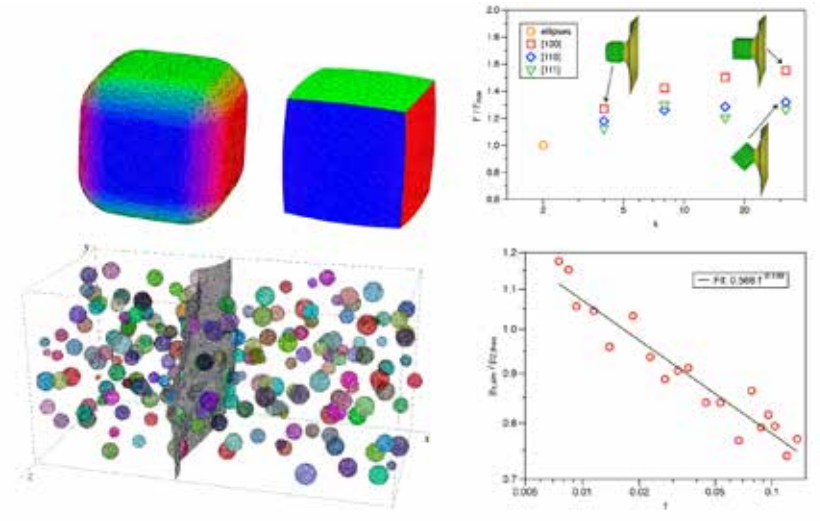
3-D front tracking model for interfaces with anisotropic energy

V. Mohles

Computational Materials Science, **176**, 109534 (2020)

A new 3-dimensional front tracking model for grain boundaries (GBs) has been developed. It allows to efficiently simulate the motion of GBs in interaction with other GBs or particles of secondary phases. The model fully accounts for the dependence of the grain boundary energy on the local orientation of the boundary plane, in the sense that any functional dependence can be chosen. In principle, this model allows to study grain growth or recrystallisation considering any realistic description of the GB energy. The present paper describes the deri- vation of the mathematical concept from basic mechanics, in particular the consideration of the Herring torque, and some implementation details.

The model is verified by comparison with analytical models. For some heuristic GB energy dependences, the equilibrium shape of a singular grain with a fixed volume embedded in another grain is calculated and discussed. As a first application, the Zener drag for realistic arrangements of about 1350 particles has been derived from simulations.



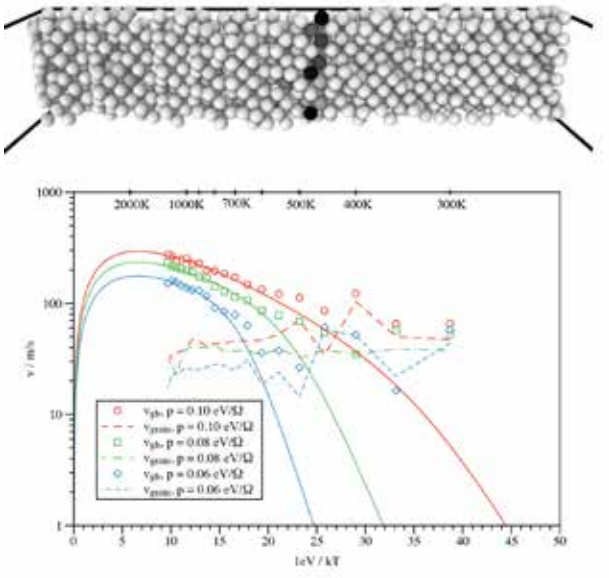
A new 3-D front tracking model for grain boundaries has been developed. It allows to efficiently simulate the motion of grain boundaries in interaction with other ones or particles of secondary phases. The model fully accounts for the boundaries' energy anisotropy. As a first application, the Zener drag for realistic particle arrays has been derived from simulations.

Efficient calculation of the ECO driving force for atomistic simulations of grain boundary motion

A. A. Schratt, V. Mohles

Computational Materials Science, **182**, 109774 (2020)

A new formulation and implementation of the Energy Conserving Orientational (ECO) Driving Force (DF) for Molecular Dynamics (MD) simulations of grain boundary (GB) motion has been developed. While the original ECO-DF slows down MD simulations of GB motion by more than an order of magnitude, the new version is almost as efficient as the widely used Janssens DF (J-DF). In order to rate the new method in comparison to others, the velocity of a symmetric Σ5 (001) 36.87° tilt GB in nickel has been simulated using the new ECO-DF and the J-DF. The deviations are discussed, including the impacts on the AIRwalk method to evaluate the GB mobility. The temperature T, the DF magnitude p, and the boundary conditions were varied. Under fully periodic boundaries, all results consistently yield a GB velocity v(p, T) that is based on two subsequent or co-dependent mechanisms, shuffling and its initiation, just like for a symmetric Σ7 (111) 38.2° tilt GB investigated previously with the original ECO-DF. Under the so-called shrink-wrapped boundary conditions, a relative grain displace- ment occurs. The magnitude of this coupling effect strongly depends on temperature. From the comparison of simulations under different boundary conditions it appears probable that the initiation process under periodic boundary conditions is actually the initiation of GB sliding, which needs to undo fully coupled grain motion. The shuffling mechanism is the combined GB motion fully coupled with grain displacement.

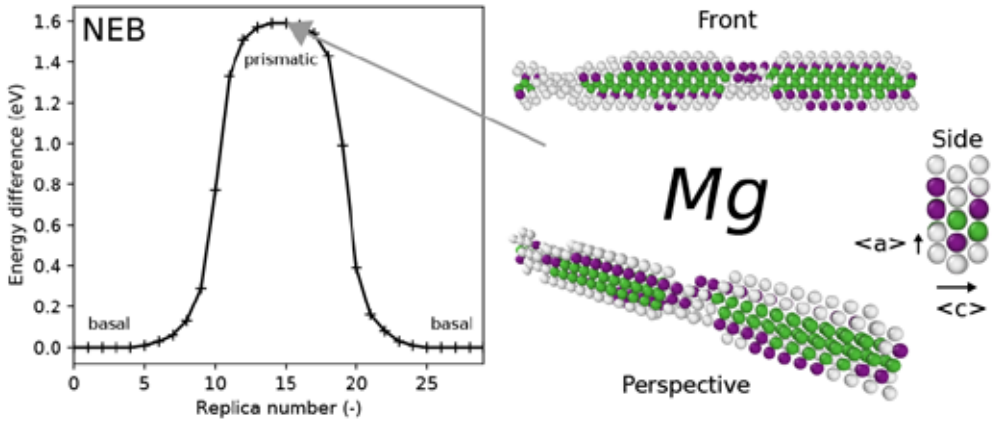


Atomistic simulations of grain boundary motion utilising a new, efficient implementation of the energy-conserving orientational driving force were performed with different boundary conditions and compared to existing methods and simulation results. Simulations with open and periodic boundary conditions differ drastically in the mechanisms of grain boundary motion.

Prismatic slip in Magnesium

M. A. Stricker, W. A. Curtin
Journal of Physical Chemistry C, **124**, 27230-27240 (2020)

Magnesium is the lowest-density structural metal but has low ductility that limits applications. The low ductility is related to the hexagonally close-packed crystal structure where activation of nonbasal slip is required for general plasticity. Here, our recent neural network potential (NNP) for Mg, trained using Kohn–Sham density functional theory (DFT), is used to examine slip of (a) dislocations on the prismatic plane. The generalized stacking fault surface energies (GSFEs) for basal and prismatic slip are computed and agree better with Kohn–Sham density functional theory (KS-DFT) than orbital-free density functional theory (OF-DFT) and modified embedded atom method (MEAM), which predict spurious minima. Consistent with the generalized stacking fault energy (GSFE), direct simulations of the prismatic (a) screw dislocation show it is unstable to dissociate into the (a) basal screw dislocation; this is mostly consistent with OF-DFT while MEAM predicts stability. Prismatic slip is thus achieved by a double-cross-slip process of the stable basal dislocations driven by a resolved shear stress on the orthogonal prismatic plane; this is consistent with the process deduced from experiments. The Nudged Elastic Band method is used with the NNP to examine the atomistic path and the stress-dependent enthalpy barrier for this mechanism; this requires many tens of thousands of atoms. The basal-prismatic cross-slip occurs in increments of c/2 via basal constriction, cross-slip on the prism plane, cross-slip back onto the basal plane, and lateral motion of the created jogs to extend the new basal dislocation. Comparisons with experimental deductions show some agreement and some notable disagreement. Resolution of the differences points toward further large-scale studies that require the accuracy and efficiency of KS-DFT-trained NNP, an approach that is also naturally extendable to the important domain of Mg alloys.

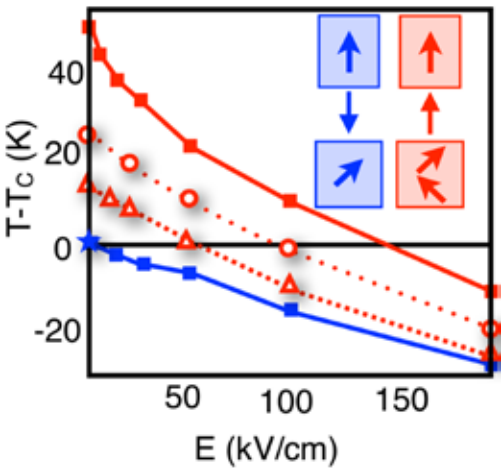


Energy difference versus normalized displacement and highest energy atomic configuration of a prismatic cross-slip process between two neighboring basal planes as determined by a nudged elastic band simulation with a neural network potential in pure Magnesium.

Impact of domains on the orthorhombic-tetragonal transition of $BaTiO_3$: An ab initio study

A. Grünebohm, M. Marathe
Physical Review Materials, **4**, 114417 (2020)

We investigate the multidomain structures in the tetragonal and orthorhombic phases of $BaTiO_3$ and the impact of the presence of domain walls on the intermediary phase transition. We focus on the change in the transition temperatures resulting from various types of domain walls and their coupling with an external electric field. We employ molecular dynamics simulations of an ab initio effective Hamiltonian in this study. After confirming that this model is applicable to multidomain configurations, we show that the phase-transition temperatures strongly depend on the presence of domains walls. Notably we show that elastic 90° walls can strongly reduce thermal hysteresis. Further analysis shows that the change in transition temperatures can be attributed to two main factors: long-range monoclinic distortions induced by walls within domains and domain wall widths. We also show that the coupling with the field further facilitates the reduction of thermal hysteresis for orthorhombic 90° walls, making this configuration attractive for future applications.

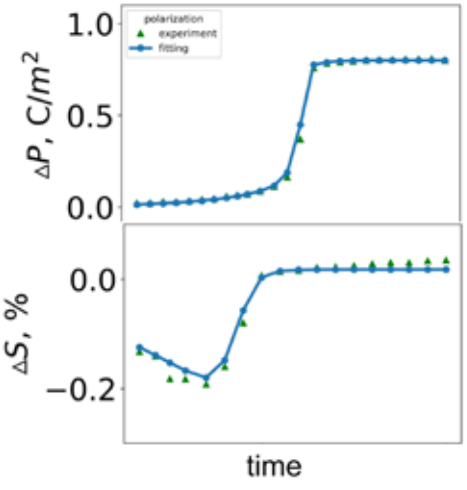


Reduction of thermal hysteresis of the the tetragonal to orthorhombic phase transition in $BaTiO_3$ with increasing density of 90° domain walls.

Multistep stochastic mechanism of polarization reversal in rhombohedral ferroelectrics

Y. A. Genenko, R. Khachaturyan, I. S. Vorotiahin, J. Schultheiß, J. E. Daniels, A. Grünebohm, J. Koruza
Physical Review B, **102**, 64107 (2020)

A stochastic model for the field-driven polarization reversal in rhombohedral ferroelectrics is developed, providing a description of their temporal electromechanical response. Application of the model to simultaneous measurements of polarization and strain kinetics in a rhombohedral $Pb(Zr,Ti)O_3$ ceramic over a wide time window allows the identification of preferable switching paths, fractions of individual switching processes, and their activation fields. In conjunction, the phenomenological Landau-Ginzburg-Devonshire theory is used to analyze the impact of an external field and stress on switching barriers, showing that residual mechanical stress may promote the fast switching.



Experimental measurements (dots) of polarization kinetics and consequent strain variation, fitted by a multistep stochastic mechanism model (solid line) with all possible switching channels (insert) for an orthorhombic symmetry.

ICAMS

Publications

16. Publications

► Publications in Refereed Journals, Proceedings, and Books

E. Anttila, D. Balzani, A. Desyatova, P. Deegan, J. Mac Taggart, A. Kamenskiy
Mechanical damage characterization in human femoropopliteal arteries of different ages
Acta Biomaterialia, 90, 2019, 225-240

S. Schmitt, M. A. Stricker, P. Gumbsch, K. Schulz
A mechanism-based homogenization of a dislocation source model for bending
Acta Materialia, 164, 2019, 663-672

D. Qiu, P. Zhao, C. Shen, W. Lu, D. Zhang, M. Mrovec, Y. Wang
Predicting grain boundary structure and energy in BCC metals by integrated atomistic and phase-field modeling
Acta Materialia, 164, 2019, 799-809

D. Gaertner, K. Abrahams, J. Kottke, V. A. Esin, I. Steinbach, G. Wilde, S. V. Divinski
Concentration-dependent atomic mobilities in FCC CoCrFeMnNi high-entropy alloys
Acta Materialia, 166, 2019, 357-370

M. Lenz, Y. M. Eggeler, J. Müller, C. H. Zenk, N. Volz, P. Wollgramm, G. Eggeler, S. Neumeier, M. Goeken, E. Spiecker
Tension/compression asymmetry of a creep deformed single crystral Co-base superalloy
Acta Materialia, 166, 2019, 597-610

A. Kwiadkowski da Silva, R. D. Kamachali, D. Ponge, B. Gault, J. Neugebauer, D. Raabe
Thermodynamics of grain boundary segregation, interfacial spinodal and their relevance for nucleation during solid-solid phase transitions
Acta Materialia, 168, 2019, 109-120

C. Meid, M. Eggeler, P. Watermeyer, A. Kostka, T. Hammerschmidt, R. Drautz, G. Eggeler, M. Bartsch
Stress-induced formation of TCP phases during high temperature low cycle fatigue loading of the single-crystal Ni-base superalloy ERBO/1
Acta Materialia, 168, 2019, 343-352

K. Hackl, A. U. Khan, F. D. Fischer, J. Svoboda
Influence of bulk energy and triple junction mobility on interface kinetics – a tool for interpretation of experiments
Acta Materialia 174, 2019, 310-318

C. Wang, M. A. Ali, S. Gao, J. V. Görler, I. Steinbach
Combined phase-field crystal plasticity simulation of P- and N-type rafting in Co-based superalloys
Acta Materialia, 175, 2019, 21-34

O. Shchyglo, G. Du, J. K. Engels, I. Steinbach
Phase-field simulation of martensite microstructure in low-carbon steel
Acta Materialia, 175, 2019, 415-425

H. Zhou, R. Hubek, M. Peterlechner, G. Wilde
Two-stage rejuvenation and the correlation between rejuvenation behavior and the boson heat capacity peak of a bulk metallic glass
Acta Materialia, 179, 2019, 308-316

I. Lopez-Galilea, B. Ruttert, J. He, T. Hammerschmidt, R. Drautz, B. Gault, W. Theisen
Additive manufacturing of CMSX-4 Ni-base superalloy by selective laser melting: influence of processing parameters and heat treatment
Additive Manufacturing, 30, 2019, 100874

F. Emeis, J. Leuthold, K. Spangenberg, M. Peterlechner, G. Wilde
Characterization of special grain boundaries and triple junctions in CuNi1-alloys upon deformation and annealing
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PhD Thesis, Ruhr-Univesität Bochum

M. Stratmann
Intergrated phase-field model with redistributation and long-range diffusion on sublattices
PhD Thesis, Ruhr-Univesität Bochum

H. J. Schaar
Simulation of solidification on the macro- and microscale in context of Ni-based superalloys
PhD Thesis, Ruhr-Univesität Bochum

ICAMS

Talks and Posters

17. Talks and Posters

▶ Invited Talks

14.01.2019
S. G. Fries
Complex phases in applied alloys: Gibbs energies modelling supported by first-principles
TU Bergakademie Freiberg, Germany

30.01.2019
R. Drautz
Development and validation of interatomic potentials and application to the simulation of phase transformations
EPFL Lausanne, Switzerland

31.01.2019
J. Neugebauer, J. Janssen, F. Körmann, T. Hickel, B. Grabowski
Exploration of large ab initio data spaces to design materials with superior mechanical properties
Physics and Theoretical Division Colloquium, Los Alamos National Laboratory, USA

05.03.2019
T. Hickel
Application of density functional theory in the context of phase diagram modelling
MSIT Winter School, Ringberg, Germany

10.03.2019
G. Wilde
Self-diffusion in high-entropy alloys
TMS Annual Meeting, San Antonio, USA

12.03.2019
I. Steinbach, M. A. Ali, J. V. Görler, O. Shchyglo
Effect of diffusion and creep on rafting of Ni-base superalloys: a phase-field study in comparison to experiments
MINES ParisTech, France

13.03.2019
J. Neugebauer, M. Todorova, B. Grabowski, T. Hickel
Modelling structural materials in realistic environments by ab initio thermodynamics
TMS Annual Meeting, San Antonio, USA

20.03.2019
G. Sutmann
Parallel computing of complex systems II
IFF Spring School 2019, Scattering! Soft, Functional and Quantum Materials, Jülich, Germany

27.03.2019
M. Mrovec
Atomistic simulations of extended defects in iron and its compounds using magnetic bond order potentials
ONERA, Paris, France

02.04.2019
T. Hickel, P. Dey, E. McEniry, M. Yao, M. Herbig, M. Lipinska-Chwalek, C. Liebscher, D. Music, B. Hallstedt, C. Haase, W. Song, C. Scheu, D. Ponge, D. Raabe, J. Neugebauer
κ carbide microstructures and the role of interfaces in high-Mn lightweight steels
High-Mn Steel 2019, Aachen, Germany

04.04.2019
T Hickel, J. Janssen, H. Sözen, F. Körmann, S. Surendralal, M. Todorova, Y. Lysogorskiy, R. Drautz, J. Neugebauer
High-throughput optimization of finite temperature phase stabilities: concepts and application
DPG Frühjahrstagung der Sektion Kondensierte Materie, Regensburg, Germany

09.04.2019
J. Neugebauer
Automizing work flows in computational materials design
Traceability and securing of results as essential challenges of research in the digital age, Berlin, Germany

15.04.2019
J. Rogal
Enhanced sampling approaches to capture atomistic processes during structural phase transformations in condensed matter systems
Physikalisches Kolloquium, Ruhr-Universität Bochum, Germany

16.04.2019
J. Rogal
A kinetic Monte Carlo study of hydrogen diffusion and thermal desorption
HEMS Workshop: Current Understanding and Future Needs, University of Oxford, UK

09.05.2019
T. Hammerschmidt
Electronic structure based descriptors of local atomic environments
ML4MS – Young Researcher's Workshop on Machine Learning for Materials Science, Aalto, Finland

13.05.2019
J. Frenzel
Introduction to shape memory and superelasticity
SMST 2019, Workshop, Konstanz, Germany

14.05.2019
I. Steinbach
Rafting of superalloys under high temperature creep conditions; multiphase-field simulation coupled to crystal plasticity
Karlsruhe Institute of Technology, Karlsruhe, Germany

14.05.2019
G. Eggeler
On the crucial role of microstructure in shape memory technology
SMST 2019, Workshop, Konstanz, Germany

14.05.2019
J. Frenzel
Recent progress on Ti-Ta shape memory alloys
SMST 2019, Workshop, Konstanz, Germany

16.05.2019
T. Hammerschmidt
Machine-learning material properties with electronic-structure based descriptors
Los Alamos National Laboratory, USA

23.05.2019
J. Neugebauer, J. Janssen, T. Hickel
Automated uncertainty analysis and quantification for high-precision DFT calculations
Workshop Precision Quantification in DFT, Louvaine-la-Neuve, Belgien

29.05.2019
J. Rogal
Path collective variables for sampling structural phase transformations
Computational mathematics for model reduction and predictive modelling in molecular and complex systems, CECAM, Lausanne, Switzerland

03.06.2019
G. Sutmann
Introduction to load balancing
E-CAM International Workshop, Jülich Supercomputing Centre, Germany

04.06.2019
T. Hickel, B. Dutta, I. Stockem, F. Körmann, J. Neugebauer
Ab initio design strategies for NiMn-based FSMA
6th International Conference of Ferromagnetic Shape-Memory Alloys CFSMA, Prague, Czech Republic

07.06.2019
J. Rogal
Enhanced sampling of atomistic processes during structural phase transformations
Colloquium of the Physics Department, Freie Universität Berlin, Germany

12.06.2019
L. Huber, R. Hadian, B. Grabowski, J. Neugebauer
Computing and modelling solute-grain boundary interaction
Canadian Materials Science Conference, Vancouver, Canada

13.06.2019
R. Janisch
Is hydrogen-enhanced decohesion at grain boundaries in ferritic steels a consequence of co-segregation? – Insights from ab-initio calculations
ALEMI workshop, Vancouver, Canada

17.06.2019
T. Hammerschmidt
From the electronic structure to materials design
Physikalisches Kolloquium, Ruhr-Universität Bochum, Germany

24.06.2019
S. V. Divinski, D. Gaertner, M. Vaidya, S. Sen, J. Kottke, A. Fareed, M. Kirschbaum, M. Garlapati, O. Lukianova, J.-F. Zhang, G. Wilde, K. Abrahams, I. Steinbach, V. Esin, B. Grabowski, X. Zhang, K. G. Pradeep, Y. Chumlyakov, M. Laurent-Brocq, L. Rogal, A. Paul, A. Pokoev
Diffusion in high-entropy alloys: myths and trues
15th International Conference on Diffusion in Solids and Liquids, Athens, Greece

26.06.2019
I. Steinbach, K. Abrahams
Generalized pair-diffusion model for multi-principal element alloys
15th International Conference on Diffusion in Solids and Liquids, Athens, Greece

27.06.2019
A. Gupta, T. Hickel, J. Neugebauer, B. Tas Kavakbasi, Y. Buranova, V. Kulitskiy, G. Wilde, S. Divinski
Precipitate-induced nonlinearities of solute diffusion in Al-based alloys
15th International Conference on Diffusion in Solids and Liquids, Athens, Greece

27.06.2019
T. Hammerschmidt
Prediction of structural stability: from structure maps to machine learning
Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

01.07.2019
S. Divinski
Grain boundary phase transformations
Interphase and intergranular boundaries (iib 2019), Paris, France

07.07.2019
G. Wilde
Shear bands in metallic glasses: atomic transport, propagation and relaxation behaviour
ISMANAM 2019, Chennai, India

08.07.2019
J. Neugebauer
Machine learning in materials: screening and discovery
Gordon Research Conference Physical Metallurgy, Coupling Computation, Data Science and Experiments in Physical Metallurgy, Manchester, USA

15.07.2019
T. Hammerschmidt
Electronic-structure based exploration of materials space
Materials Science Colloquium, Institute of Materials Science, Universität Stuttgart, Germany

24.07.2019
J. Rogal
Path collective variables for enhanced sampling of structural phase transformations
Car-Parrinello Molecular Dynamics 2019 – Pushing the Boundaries of Molecular Dynamics, EPFL/CECAM, Lausanne, Switzerland

01.08.2019
R. Drautz
Atomistic simulations for alloy development
Los Alamos National Laboratory, USA

05.08.2019
J. Neugebauer, L. Huber, F. Körmann, B. Grabowski, T. Hickel
Ab initio input for multiphysics models: accuracy, performance and challenges
ISAM4: The fourth International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

07.08.2019
J. Rogal
Enhanced sampling of phase boundary migration
International Symposium on Atomistic and Multi-scale Modeling of Mechanics and Multiphysics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

14.08.2019
G. Díaz Leines
Rare events sampling: unraveling the atomistic mechanisms and kinetics of complex systems
National Autonomous University of Mexico, Mexico City

19.08.2019
G. Sutmann
Multi-level load balancing for particle simulation methods
Los Alamos National Laboratory, USA

20.08.2019
I. Steinbach, J. Kundin
de Broglie Bohm double solution program reloaded: doublon network in 1+1+2 dimensions
Energy Materials Nanotechnology 2019, Barcelona, Spain

22.08.2019
G. Díaz Leines, J. Rogal
Shedding light on the atomistic mechanisms of polymorph selection during crystal nucleation in metal alloys
XXVIII International Materials Research Congress, Cancún, Mexico

01.09.2019
R. Janisch, J. Möller, E. Bitzek, H. u. Hassan, A. Hartmaier
Segregation and embrittlement at grain boundaries in multicomponent steel - insights from ab-initio calculations
EUROMAT 2019, Stockholm, Sweden

04.09.2019
J. Neugebauer
Ab initio guided materials design and discovery
Inaugural Symposium for Computational Materials, Skoltech, Moscow, Russia

09.09.2019
T Hickel, J. Janssen, H. Sözen, F. Körmann, J. Neugebauer, Y. Lysogorskiy, R. Drautz
Ab initio simulation of finite temperature phase stabilities: concepts and application
HetSys Launch Event, Warwick, UK

10.09.2019
J. Neugebauer
Ab initio description of coupling phenomena between magnetic and structural degrees of freedom
EASTMAG2019, Jekaterinburg, Russia

13.09.2019
F. Varnik
Modelling shape memory polymers: from molecular understanding towards engineering applications
Covestro Deutschland AG, Leverkusen, Germany

20.09.2019
Y. Lysogorskiy
Applied machine learning in materials science: overview and case studies
Advanced Functional Materials Laboratory, Linköping University, Sweden

30.09.2019
T. Hammerschmidt
Electronic structure based descriptors of local atomic environments
Machine Learning and Informatics for Chemistry and Materials, Telluride Science Research Center, Colorado, USA

01.10.2019
F. Körmann, Y. Ikeda, P. Srinivasan, J. Neugebauer, B. Grabowski, T. Kostiuchenko, A. Shapeev
Phase stability and mechanical properties of high entropy and chemically complex alloys
MS&T, Portland, USA

03.10.2019
J. Rogal
Extended timescale simulations of structural phase transformations in materials
Aalto Physics Research Seminar, Aalto University, Helsinki, Finland

28.10.2019
Y. Lysogorskiy, T. Hammerschmidt, R. Drautz
Data-driven approach for the validation of interatomic potentials
Thermodynamics and Kinetics Group, NIST, Gaithersburg, USA

28.10.2019
J. Rogal
Extended timescale simulations of structural phase transformations in materials
Warwick Centre for Predictive Modelling Seminar, University of Warwick, Coventry, UK

29.10.2019
G. Sutmann
Multi-level load balancing for particle simulation methods
Particles Conference 2019 VI International Conference on Particle-Based Methods, Barcelona, Spain

31.10.2019
Y. Lysogorskiy, T. Hammerschmidt, R. Drautz
Data-driven approach for the validation of interatomic potentials
Department of Aerospace Engineering Mechanics, University of Minnesota, Minneapolis, USA

18.11.2019
J. Rogal
Enhanced sampling of atomistic processes during structural phase transformations
Institute of Materials, EPFL, Lausanne, Switzerland

18.11.2019
A. Grünebohm
New concepts for cooling: origins of the inverse electrocaloric effect
Physikalisches Kolloquium, Ruhr-Universität Bochum, Germany

20.11.2019
J. Neugebauer, J. Janssen, F. Körmann, T. Hickel, B. Grabowski
Ab initio descriptors to design materials with superior mechanical properties
Materials Day, ETH Zürich, Switzerland

21.11.2019
A. Hartmaier
Atomistically informed continuum models for deformation and failure of materials
Integrated Computation Materials, Process and Product Engineering, Leoben, Austria

09.12.2019
Y. Lysogorskiy, T. Hammerschmidt, M. Mrovec, R. Drautz
Data management for atomistic simulations: design and case studies
Materials Integration International Workshop, National Institute for Materials Science, Tsukuba, Japan

09.12.2019
J. Neugebauer
Machine learning in materials: screening and discovery
National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

09.12.2019
I. Roslyakova
Artificial materials intelligence
The 47th MaDIS Seminar SIP-Materials Integration International Workshop in NIMS, Sengen, Japan

09.12.2019
I. Steinbach
High temperature creep of Ni and Co-base superalloys: integration of physics based simulation and machine-learning
The 47th MaDIS Seminar ,SIP-Materials Integration International Workshop in NIMS, Sengen, Japan

09.12.2019
S. Zomorodpoosh
Modeling strategy for creep behavior of Co-base superalloys
The 47th MaDIS Seminar SIP-Materials Integration International Workshop in NIMS, Sengen, Japan

11.12.2019
J. Neugebauer, J. Janssen, F. Körmann, T. Hickel, B. Grabowski
Construction and exploitation of large ab initio data spaces to design materials with superior mechanical properties
Materials Research Meeting 2019, Yokohama, Japan

12.12.2019
Y. Lysogorskiy, T. Hammerschmidt, M. Mrovec, R. Drautz
Data management for atomistic simulations: design and case studies
Materials Research Meeting 2019, Yokohama, Japan

12.12.2019
I. Steinbach, M. Ahmed, M. A. Ali, I. Roslyakova
3-D phase-field simulations to machine-learn 3-D features from 2-D microstructure
Materials Research Meeting 2019, Yokohoma, Japan

12.12.2019
I. Roslyakova
Artificial materials intelligence
Materials Research Meeting 2019, Yokohoma, Japan

19.12.2019
J. Frenzel
Neue Entwicklungen im Bereich der Elektronenrückstreubeugung
Jahresabschluss-Symposion des Instituts für Werkstoffe, Ruhr-Universität Bochum, Germany

15.01.2020
T. Hickel, U. Aydin, H. Sözen, B. Dutta, Z. Pei, J. Neugebauer
Innovative concepts in materials design to boost renewable energies
Seminar des Institute for Innovative Technologies an der SRH Hochschule Berlin, Germany

15.01.2020
Y. Lysogorskiy
Data-driven approach: current research activities and methods
Westfälische Wilhelms-Universität Münster, Germany

21.01.2020
T. Hickel, E. McEniry, R. Nazarov, P. Dey
Ab initio basierte Simulation zur Wasserstoff-versprödung in hoch-Mn Stählen
Seminar der Staatlichen Materialprüfungsanstalt Darmstadt, Institut für Werkstoffkunde, Darmstadt, Germany

21.01.2020
J. Frenzel
Cross-correlation EBSD und high-quality Kikuchi-pattern – Neue Entwicklungen im Bereich der Elektronenrückstreubeugung
TU Chemnitz, Germany

18.02.2020
T. Hickel
Application of density functional theory in the context of phase diagram modelling
MSIT Winter School, Ringberg, Germany

23.02.2020
G. Wilde
Self-diffusion in high-entropy alloys: the impact of constituents and composition
TMS Annual Meeting, San Diego, USA

24.02.2020
J. Frenzel, P. Hallenleben, F. Scholz, P. Thome, G. Eggeler
Crystal mosaicity in single crystal Ni-based superalloys
TMS Annual Meeting, San Diego, USA

24.02.2020
T. Hammerschmidt
Thermodynamic modelling of precipitates of topologically close-packed phases
TMS Annual Meeting, San Diego, USA

26.02.2020
G. Eggeler
Early nanoscale dislocation processes and two creep rate minima in SX Ni-base superalloys
TMS Annual Meeting, San Diego, USA

27.02.2020
F. Körmann, Y. Ikeda, P. Srinivasan, B. Dutta, J. Neugebauer, B. Grabowski, T. Kostiuchenko, A. Shapeev
Ab initio phase stabilities of high entropy and chemically complex alloys
TMS Annual Meeting, San Diego, USA

27.02.2020
J. Neugebauer, J. Janssen, L. Huber, Y. Ikeda, F. Körmann, B. Grabowski, T. Hickel, A. Shapeev
Materials design in high dimensional chemical and structural configuration spaces
TMS Annual Meeting, San Diego, USA

23.06.2020
G. Sutmann
Hierarchical load-balancing for particle- and mesh-based simulations
Computational Science Division Seminar, Jülich Supercomputing Centre, Germany

29.06.2020
R. Drautz
Atomic cluster expansion for accurate and transferable interatomic potentials
Modern Approaches to Coupling Scales in Materials Simulations Workshop, Technische Universität München, Germany

09.07.2020
T. Hammerschmidt
Machine-learning material properties with domain knowledge of the interatomic bond
Exploiting Machine Learning in Multiscale Modelling of Materials, Warwick, UK

24.07.2020
G. Eggeler
Towards a new generation of superalloy single crystals – creep strength, the importance of early nanoscale dislocation processes and the role of dislocations in microstructural evolution
MSE 2020 Plenary Lecture, Online Event

22.09.2020
R. Drautz
From electrons to interatomic potentials for materials simulation
Autumn School on Correlated Electrons, Forschungszentrum Jülich, Germany

28.09.2020
G. Wilde
Fast Scanning Chip calorimetry: new measurement capabilities at high controlled rates
17th Discussion Meeting on Thermodynamics of Alloys (TOFA), Bad Staffelstein, Germany

09.10.2020
R. Drautz
Atomic cluster expansion for accurate and transferable interatomic potentials
HQS Seminars, Seevetal-Ramelsloh, Germany

14.10.2020
G. Sutmann, M. Longsworth, H. Ganesan
Simulation of segregation in parallel hybrid MD/MC simulations
Conference on Computational Physics, Moscow, Russia

02.11.2020
S. Divinski
Grain boundary phase transformations probed by diffusion measurements
ADIS Workshop (Ab-Initio Description of Iron and Steel) 2020, Online Workshop

04.11.2020
R. Janisch, A. Azócar Guzmán, X. Huang, J. Jeon
Hydrogen-enhanced decohesion at grain boundaries in ferritic steels
ADIS Workshop (Ab-Initio Description of Iron and Steel) 2020, Online Workshop

29.11.2020
G. Wilde
Coupling between MRO structure and local plasticity of metallic glasses
MRS Fall Meeting, Boston, USA

▶ Contributed Talks and Posters

09.01.2019
A. Ferrari, D. G. Sangiovanni, J. Rogal, R. Drautz
First principles characterization of reversible transformations in shape memory alloys
19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste, Italy

14.01.2019
G. Díaz Leines, J. Rogal
Maximum likelihood analysis of reaction coordinates during solidification in Ni
Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials, Trieste, Italy

14.02.2019
D. Bürger, G. Eggeler
Doppelscherkriechversuche an einkristallinen Nickelbasis-Superlegierungen
Gefüge und Bruch 2019, Bochum, Germany

14.02.2019
M. Schneider, G. Eggeler
Einfluss des Gefüges auf die mechanischen Eigenschaften der CrCoNi Medium-Entropie-legierungen
Gefüge und Bruch 2019, Bochum, Germany

14.02.2019
L. Cao, G. Eggeler
Kriechversuche an Proben mit Rundkerben aus einkristallinen Ni-Basis Superlegierungen
Gefüge und Bruch 2019, Bochum, Germany

14.02.2019
G. Eggeler
Mikro- und Makroscherversuche an einkristallinen Ni-Basis Superlegierungen
Gefüge und Bruch 2019, Bochum, Germany

14.02.2019
G. Laplanche, A. Asabre, G. Eggeler
Widmanstätten-Gefüge und Versagensverhalten von chemisch komplexen Legierungen
Gefüge und Bruch 2019, Bochum, Germany

14.02.2019
O. Horst, G. Eggeler
Zum Einfluss von HIP-Behandlungen auf die Kriechlebensdauer von einkristallinen Ni-Basis Superlegierungen
Gefüge und Bruch 2019, Bochum, Germany

19.02.2019
J. K. Engels, N. Vajragupta, A. Hartmaier
Inverse analysis on tempered lath martensite: a materials science and methodological study
Nanobrücken 2019, Berlin, Germany

24.02.2019
B. Tas-Kavakbasi, F. Emeis, V. Kulitcki, S. V. Divinski, G. Wilde
Effect of shear strain on the microstructure of Al-Sc-Zr-based alloy
Euromat 2019, Stockholm, Sweden

24.02.2019
A. Gupta, Y. Buranova, V. Kulitcki, K. Li, Y. Du, B. Dutta, T. Hickel, J. Neugebauer, G. Wilde, S. V. Divinski
Thermodynamics and kinetics of precipitate formation in Al-Sc-Zr alloys: theory and experiments
Euromat 2019, Stockholm, Sweden

01.03.2019
Y. Lysogorskiy, T. Hammerschmidt, R. Drautz
Data management and high-throughput workflows for atomistic simulations
Multiscale Materials Simulation and Materials Integration, Bochum, Germany

25.03.2019
Y. Lysogorskiy, A. Ferrari, R. Drautz
Data-driven methods for multi-principal element alloys discovery
General Meeting of DFG Priority Programme Compositionally Complex Alloys - High Entropy Alloys, KIT, Karlsruhe, Germany

01.04.2019
Y. Lysogorskiy, T. Hammerschmidt, R. Drautz
Validation and transferability of interatomic potentials
DPG Spring Meeting, Regensburg, Germany

02.04.2019
A. Azócar Guzmán, R. Janisch, A. Hartmaier
Size independent description of the strain effects on the segregation of carbon and hydrogen in iron
DPG Spring Meeting, Regensburg, Germany

02.04.2019
R. Janisch, X. Huang, A. Hartmaier
Partitioning of segregating impurities during grain boundary decohesion
DPG Spring Meeting, Regensburg, Germany

02.04.2019
G. Díaz Leines, J. Rogal
Atomistic mechanism of nucleation in Ni: the role of pre-structuring and seeding in polymorph selection
DPG Spring Meeting, Regensburg, Germany

02.04.2019
S. Starikov, M. Mrovec, R. Drautz
Atomistic simulations of bulk and grain boundary diffusion in bcc iron
DPG Spring Meeting, Regensburg, Germany

02.04.2019
Y. Liang, G. Díaz Leines, J. Rogal, R. Drautz
Atomistic study of nucleation and growth in Ni3Al
DPG Spring Meeting, Regensburg, Germany

03.04.2019
A. Ferrari, D. G. Sangiovanni, J. Rogal, R. Drautz
An ab initio perspective on the reversible martensitic transformation in Ti-Ta shape memory alloys
DPG Spring Meeting, Regensburg, Germany

03.04.2019
D. Smirnova, Y. Liang, G. Díaz Leines, S. Starikov, N. Wang, M. Popov, D. G. Sangiovanni, I. Abrikosov, R. Drautz, M. Mrovec
Atomistic description of self-diffusion in molybdenum
DPG Spring Meeting, Regensburg, Germany

03.04.2019
A. Ferrari, M. F. Schröder, Y. Lysogorskiy, J. Rogal, M. Mrovec, R. Drautz
Parametrization of a bond-order potential for Ti
DPG Spring Meeting, Regensburg, Germany

04.04.2019
T. Pradhan, A. Kholtobina, L. Romaner, M. Mrovec, R. Drautz
Atomistic simulations of mixed ½ [111] dislocations in bcc transition metals
DPG Spring Meeting, Regensburg, Germany

18.04.2019
R. Janisch
Is hydrogen-enhanced decohesion at grain boundaries in ferritic steels a consequence of co-segregation? – Insights from ab-initio calculations
Hydrogen in metals – current understanding and future needs, Oxford, United Kingdom

06.05.2019
J. Frenzel, A. Wiczorek, G. Eggeler
Kühlen mit Formgedächtnislegierungen
Bokomat 2019, Ruhr-Universität Bochum, Germany

21.05.2019
Y. Lysogorskiy, T. Hammerschmidt, R. Drautz
Data-driven approach for the validation of interatomic potentials
ICAMS Advanced Discussions, Bochum, Germany

21.05.2019
N. Vajragupta, A. Biswas,
M. Ramaswamy Guru Prasad, A. Hartmaier
Data-driven toolkit for property-based design of microstructures
ICAMS Advanced Discussions, Bochum, Germany

27.05.2019
Y. Liang, G. Díaz Leines, J. Rogal, R. Drautz
Atomistic simulation of nucleation process in binary alloy Ni3Al
IMPRS-SurMat Retreat, Kreuth, Germany

28.05.2019
T. Pradhan, A. Kholtobina, L. Romaner, M. Mrovec,
R. Drautz
Atomistic simulations of mixed ½ [111] dislocations in bcc transition metals
IMPRS-SurMat Retreat, Kreuth, Germany

03.06.2019
A. Obaied, S. Zomorodpoosh, I. Roslyakova,
I. Steinbach
Third generation CALPHAD database from 0K up to 6000K for 8 transition elements
CALPHAD XLVIII, Singapore

04.06.2019
N. H. Paulson, S. Zomorodpoosh, I. Roslyakova,
M. Stan
Automated weighting of data in CALPHAD – a comparison between frequentist and Bayesian approaches
CALPHAD XLVIII, Singapore

04.06.2019
I. Roslyakova, A. Müller, S. Zomorodpoosh,
C. Koerner, I. Steinbach
Role of materials informatics in computer-based design of Ni-/Co-based single crystal superalloys
CALPHAD XLVIII, Singapore

05.06.2019
A. Obaied, S. Zomorodpoosh, I. Roslyakova, L. Zhang
Thermodynamic re-assessment of pure chromium using modified segmented regression model
CALPHAD XLVIII, Singapore

05.06.2019
Y. Liang, G. Díaz Leines, J. Rogal, R. Drautz
Finding the reaction coordinates for crystal nucleation in Ni3Al from transition path sampling simulations
Materials Simulation Days, Mainz, Germany

07.06.2019
G. Díaz Leines, J. Rogal
Maximum likelihood analysis of reaction coordinates during crystal nucleation in Ni
Materials Simulation Days, Mainz, Germany

12.06.2019
R. Janisch, J. Möller, E. Bitzek, H. u. Hassan,
A. Hartmaier
Fracture ab initio: a force-based scaling law for atomistically informed continuum models
Canadian Materials Science Conference, Vancouver, Canada

26.06.2019
K. Abrahams, I. Steinbach
Automated assessment of atomic mobilities
15th International Conference on Diffusion in Solids and Liquids, Athens, Greece

16.07.2019
A. Grünebohm, M. Marathe
Interplay of domain structure, phase transitions and functional responses
$F^2c\pi^2$ joint conference, Lausanne, Switzerland

22.07.2019
M. Ahmed, N. Volz, M. Ali, S. Neumeier, I. Roslyakova, I. Steinbach
Image-based microstructure-property analysis using machine learning techniques supported by phase-field simulations
The 4th International Symposium on Phase-Field Modelling in Materials Science, Ruhr-Universität Bochum, Germany

24.07.2019
W. Amin, M. A. Ali, O. Shchyglo
Micromechanical modeling of metals using strain gradient plasticity-phase field method
The 4th International Symposium on Phase-Field Modelling in Materials Science, Ruhr-Universität Bochum, Germany

24.07.2019
H. F. Salama, O. Shchyglo, I. Steinbach
The effects of energy anisotropy on grain boundary characteristics during grain growth
The 4th International Symposium on Phase-Field Modelling in Materials Science, Ruhr-Universität Bochum, Germany

05.08.2019
A. Neogi, A. Hartmaier, R. Janisch
Atomistic simulation of fracture in lamellar TiAl microstructures
The 4th International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics of Materials (ISAM4), Erlangen, Germany

05.08.2019
T. Pradhan, A. Kholtobina, L. Romaner, M. Mrovec, R. Drautz
Atomistic simulations of mixed ½ [111] dislocations in bcc transition metals
The 4th International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics of Materials (ISAM4), Erlangen, Germany

05.08.2019
M. Mrovec, S. Starikov, R. Drautz
Atomistic simulations of the iron – chromium system
The 4th International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics of Materials (ISAM4), Erlangen, Germany

06.08.2019
A. Neogi, R. Janisch, A. Hartmaier
Atomistic simulation of fracture in lamellar TiAl microstructures
The 4th International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics of Materials (ISAM4), Erlangen, Germany

14.08.2019
G. Sutmann, R. Halver
A load balancing library for particle simulations – ALL
LAMMPS User Workshop, Albuquerque, USA

22.08.2019
R. Janisch, J. Möller, E. Bitzek, H. u. Hassan, A. Hartmaier
Atomistic aspects of deformation and fracture
„DCMS MATERIALS 4.0 summer school Deep Mechanics, Dresden, Germany"

12.09.2019
G. Díaz Leines, J. Rogal
Maximum likelihood analysis of reaction coordinates during crystal nucleation in Ni
CECAM 50 Years, Lausanne, Switzerland

16.09.2019
M. Mrovec, S. Starikov, R. Drautz
Atomistic simulations of dislocations in iron-chromium alloys
Dislocations 2019, Haifa, Israel

16.09.2019
T. Pradhan, A. Kholtobina, L. Romaner, M. Mrovec, R. Drautz
Core structure and mobility of mixed ½ [111] dislocations in bcc metals
Dislocations 2019, Haifa, Israel

16.09.2019
R. Khachaturyan, A. Grünebohm
Scalebridging simulation of functional composites
Materials Chain Early Career Researchers' Forum, TU Dortmund, Germany

16.09.2019
Y. Lysogorskiy, A. Ferrari, R. Drautz
Data-guided approach for multi-principal element alloys discovery
Theory of Complex Disorder in Materials, Linköping, Sweden

21.10.2019
D. Bürger, A. Parsa, M. Ramsperger, C. Körner, G. Eggeler
Creep properties of single crystal Ni-base superalloys (SX) produced by selective electron beam melting (SEBM)
EPRI-123HiMAT 2019, Nagasaki, Japan

21.10.2019
Y. Liang, G. Díaz Leines, J. Rogal, R. Drautz
Identifying a multi-dimensional reaction coordinate for the nucleation in binary Ni_3Al
3rd German-Dutch Workshop on Computational Materials Science, Domburg, Netherlands

24.10.2019
D. Smirnova, Y. Liang, G. Díaz Leines, S. Starikov, N. Wang, M. Popov, D. G. Sangiovanni, I. Abrikosov, R. Drautz, M. Mrovec
Atomistic description of self-diffusion in molybdenum
3rd German-Dutch Workshop on Computational Materials Science, Domburg, Netherlands

24.10.2019
G. Díaz Leines, J. Rogal
Atomistic mechanism of nucleation in Ni: the role of pre-structuring and seeding in polymorph selection
3rd German-Dutch Workshop on Computational Materials Science, Domburg, Netherlands

30.10.2019
S. Schulz, G. Sutmann
A consistent boundary method for the material point method - using image particles to reduce boundary artefacts
Particles 2019 VI International Conference on Particle-Based Methods, Barcelona, Spain

13.11.2019
M. Ramaswamy Guru Prasad, A. Biswas, N. Vajragupta, A. Hartmaier
Kanapy: A tool for generating complex synthetic polycrystalline microstructures
Arbeitskreise Mikrostrukturmechanik im FA Materials Modelling, Simulation and Data, Siegen, Germany

13.11.2019
A. Biswas, N. Vajragupta, R. Hielscher, A. Hartmaier
Optimal reconstruction of crystallographic texture with a reduced set of orientations
Arbeitskreise Mikrostrukturmechanik im FA Materials Modelling, Simulation and Data, Siegen, Germany

21.11.2019
I. Roslyakova
The third generation CALPHAD databases: comparison of existing modeling approaches
French-German Workshop on Thermodynamics and Kinetics, ICMPE, Thiais, France

21.11.2019
A. Obaied, S. Zomordpoosh, I. Roslyakova
Third generation CALPHAD database from 0K to 6000K for 8 transition elements
French-German Workshop on Thermodynamics and Kinetics, ICMPE, Thiais, France

02.12.2019
W. Amin, M. A. Ali, A. Hartmaier, I. Steinbach
Creep and strengthening through interfaces explained by dislocation-based strain-gradient crystal plasticity-phase field method
MRD's 2nd Young Materials Researchers Day, Ruhr-Universität Bochum, Germany

02.12.2019
H. Dumlu, A. Marquardt, K. Neuking, G. Eggeler
On the influence of small molecules triggering the one-way effect in shape-memory polymers
MRD's 2nd Young Materials Researchers Day, Ruhr-Universität Bochum, Germany

04.12.2019
D. Bürger, G. Eggeler
Doppelscherkriechversuche an einkristallinen Nickelbasis-Superlegierungen
Werkstoffprüfung 2019, Ulm, Germany

11.12.2019
N. Vajragupta, A. Biswas,
M. Ramaswamy Guru Prasad, A. Hartmaier
Mechanical property prediction of additively manufactured metals by micromechanical modelling
Materials Science and Technology of Additive Manufacturing (MSTAM), Bremen, Germany

30.01.2020
I. Roslyakova, S. Zomorodpoosh, M. Ali, A. Obaied, M. Ahmed, I. Steinbach
Data mining and machine learning applied to thermodynamic and mechanical properties of superalloys
Superalloy Data Science, Ruhr-Universität Bochum, Germany

31.01.2020
T. Hammerschmidt, A. P. Subramanyam, J. Jenke, A. Bialon, A. C. Ladines, J. Koßmann, Y. Lysogorskiy, R. Drautz
Predicting structural stability with data mining and machine learning
Superalloy Data Science, Ruhr-Universität Bochum, Germany

24.02.2020
D. Bürger, A. Parsa, M. Ramsperger, C. Körner, G. Eggeler
A comparison of creep properties between conventionally cast and additive manufactured CMSX-4
TMS 2020, San Diego, USA

24.02.2020
L. Heep, C. Schwalbe, C. Heinze, A. Dlouhy, C. Rae, G. Eggeler
Analysis of the APB energy in an additive manufactured polycrystalline Ni-based superalloy with high ?' volume fraction
TMS 2020, San Diego, USA

24.02.2020
P. Thome, S. Medgalchi, F. Scholz, G. Eggeler, J. Frenzel
Using the new rotation vector base line electron back scatter diffraction (RVB-EBSD) method to characterize single crystal cast microstructures
TMS 2020, San Diego, USA

25.02.2020
F. Scholz, D. Kotzem, P. Thome, J. Frenzel, G. Eggeler
3D characterization of the evolution of crystal mosaicity during solidification of single crystal Ni-based superalloys
TMS 2020, San Diego, USA

25.02.2020
M. Schneider, E. George, T. Záležák, A. Dlouhý, G. Eggeler, G. Laplanche
Analysis of strengthening due to grain boundaries and annealing twin boundaries in the CrCoNi medium-entropy alloy
TMS 2020, San Diego, USA

25.02.2020
A. Marquardt, K. Neuking, G. Eggeler
How small molecules can trigger the one-way effect in shape memory polymers
TMS 2020, San Diego, USA

27.02.2020
O. Horst, B. Ruttert, D. Bürger, L. Heep, H. Wang, A. Dlouhy, W. Theisen, G. Eggeler
On the rejuvenation of crept Ni-base single crystal superalloys (SX) by hot isostatic pressing (HIP)
TMS 2020, San Diego, USA

06.05.2020
H. F. Salama, K. Marquardt, J. Kundin, O. Shchyglo, I. Steinbach
The role of grain boundary energy anisotropy on the grain size evolution during normal grain growth
European Geosciences Union (EGU) general assembly, Online-meeting

27.05.2020
H. Sajjad, H. u. Hassan, M. Kuntz, B. J. Schaefer, P. Sonnweber-Ribic, A. Hartmaier
An inverse method to determine fatigue properties of materials using cyclic Vickers indentation and numerical simulation
4th International Symposium on Fatigue Design and Material Defects, Potsdam, Germany

30.06.2020
M. Shahmardani Firouzjah, P. Stahle, S. Kao-Walter
On buckling and fracture of thin elastic-plastic foils
1st Virtual European Conference on Fracture, Online event

06.08.2020
Y. Lysogorskiy
The platform for the interatomic potentials validation
NIST Atomistic Simulations for Industrial Needs Workshop, Gaithersburg, USA

10.09.2020
A. Dimou
Optimizing the electrocaloric effect in (Ba,Sr) TiO_3 with molecular dynamics simulations
5th Grandmaster Early-Career Workshop in Physics (GEWP) 2020, Prague, Czech Republic

22.09.2020
M. Ramaswamy Guru Prasad, A. Biswas, N. Vajragupta, A. Hartmaier
Influence of porosity on plasticity and damage of SLM manufactured metal assessed by a micromechanical modeling scheme
Materials Science and Engineering Congress 2020 Online Conference, TU Darmstadt, Germany

22.09.2020
A. Neogi, A. Hartmaier, R. Janisch
Orientation-dependent fracture behaviour of single crystal and two-phase intermetallic TiAl
Materials Science and Engineering Congress 2020 Online Conference, TU Darmstadt, Germany

22.09.2020
B. Tas, V. Kulitcki, A. Gupta, M. Peterlechner, J. Neugebauer, G. Wilde, T. Hickel, S. V. Divinski
Microstructure evolution of an Al-Sc-Zr-based alloy as a result of mechano-chemical coupling
Materials Science and Engineering Congress 2020 Online Conference, TU Darmstadt, Germany

23.09.2020
R. Khachaturyan
Investigation of a correlated nucleation and polarization kinetics in $BaTiO_3$ by means ab initio based molecular dynamics simulations
Materials Science and Engineering Congress 2020 Online Conference, TU Darmstadt, Germany

24.09.2020
A. Azócar Guzmán, J. Jeon, A. Hartmaier, R. Janisch
Ab initio analysis of hydrogen solution, segregation and embrittlement at cleavage plains and at a grain boundary in ferritic steel
Materials Science and Engineering Congress 2020 Online Conference, TU Darmstadt, Germany

24.09.2020
A. Grünebohm
Ab initio based optimization of functional ferroelectrics
Materials Science and Engineering Congress 2020 Online Conference, TU Darmstadt, Germany

27.09.2020
I. Roslyakova, S. Zomorodpoosh, A. Obaied, I. Steinbach
Artificial materials intelligence to accelerate discovery of novel superalloys
17th Discussion Meeting on Thermodynamics of Alloys (TOFA), Bad Staffelstein, Germany

30.09.2020
I. Roslyakova, A. Obaied, S. Zomorodpoosh
3G TDB software for automated generation of TDB files using modified segmented regression (MSR) model: pure Mn as an example
17th Discussion Meeting on Thermodynamics of Alloys (TOFA), Bad Staffelstein, Germany

01.10.2020
A. Obaied, F. Tang, I. Roslyakova, M. to Baben
2 ½ generation CALPHAD databases: experopolating heat capacities of elements and compounds to 0K
17th Discussion Meeting on Thermodynamics of Alloys (TOFA), Bad Staffelstein, Germany

01.10.2020
I. Roslyakova, A. Obaied, S. Zomorodpoosh
Application of machine learning methods to support the development of the 3d generation CALPHAD databases
17th Discussion Meeting on Thermodynamics of Alloys (TOFA), Bad Staffelstein, Germany

ICAMS

Seminars and other Lectures

18. Seminars and other Lectures

▶ Joint Seminar Series of ICAMS and the Institute for Materials

10.01.2019
Reactive magnetron sputter deposition of thin films : an overview of experiments at DRAFT, University Ghent
D. Depla
Ghent University, Belgium

24.01.2019
Adaptive isogeometric phase-field modelling of fracture
M. Kästner
TU-Dresden, Germany

31.01.2019
Solute segregation and intergranular embrittlement
P. Lejcek
Czech Academy of Sciences, Prague, Czech Republic

11.04.2019
Multiphasefield modeling on mesoscopic length scale: application to martensitic phase transformation and crack propagation
D. Schneider
Karlsruhe Institute of Technology (KIT), Karsruhe, Germany

09.05.2019
Developing alloys for service in jet engines
D. Dye
Imperial College, London, UK

16.05.2019
Fatigue ab initio
S. Schmauder
Universität Stuttgart, Germany

23.05.2019
Recent developments of Ni-Ti-Zr and Ni-Mn-Ga high-temperature shape memory alloys
J. Pons Morro
University of the Balearic Islands, Palma de Mallorca, Spain

04.07.2019
Advanced intermetallic titanium aluminides – from fundamentals to application
S. Mayer
Montanuniversität Leoben, Austria

11.07.2019
Advanced powder metallurgical methods for fabrication of metal matrix composites with tailored properties
T. Weißgärber
Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung IFAM, Dresden, Germany

31.10.2019
Scale-bridging computational design of multifunctional ferroelectric composites
A. Grünebohm
Universität Duisburg-Essen, Duisburg, Germany

21.11.2019
Challenges of cellular blood flow modelling in health (and disease)
T. Krüger
University of Edinburgh, United Kingdom

05.12.2019
Dislocation-based functionality in oxides
J. Rödel
TU Darmstadt, Germany

12.12.2019
Molecular dynamics simulations of nano-indentation and nanoscratching of metals and metal oxides
N. Gunkelmann
TU Clausthal, Germany

23.01.2020
Magnetic shape memory alloys for energy harvesting
M. Kohl
Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

29.10.2020
Multiphysics analysis of tunable electromagnetic metasurfaces
D. Chigrin
RWTH Aachen, Germany

12.11.2020
X-ray non-destructive testing of materials and composites
A. Waske
Bundesanstalt für Materialforschung (BAM), Berlin, Germany

19.11.2020
Mapping phase transformation pathways in materials and linking it to processing-micro-structure-property relationships
A. Devaraj
Pacific Northwest National Laboratory, Richland, USA

26.11.2020
Understanding the effects of stress orientation – propagation of superlattice stacking faults in Ni-based superalloys
F. D. León-Cázares
University of Cambridge, UK

► Seminars and other Lectures

13.02.2019
Atomistic studies of effect of interface curvature on misfit dislocation networks
H. Lyu
Friedrich-Alexander-Universität Erlangen Nürnberg, Germany

27.03.2019
Thermophysical and mechanical properties of Co/Ni-based superalloys
C. Zenk
The Ohio State University, Columbus, USA

10.04.2019
Developing the NIST Materials Resource Registry for sharing and discovery of materials data
C. A. Becker
US National Institute of Standards and Technology, Gaithersburg, USA

17.05.2019
Reverse non-equilibrium molecular dynamics simulations of silicon phononic crystals
R. Meyer
Laurentian University, Sudbury, Canada

03.06.2019
Denoising of EBSD data using MTEX
R. Hielscher
TU Chemnitz, Germany

04.06.2019
Modeling of polarization kinetics of ferroelectric ceramics
R. Khachaturyan
TU Darmstadt, Germany

04.06.2019
Effects of dissolved hydrogen on dislocation velocity in iron: implications for hydrogen enhanced localised plasticity
A. T. Paxton
Queen's University, Belfast, UK

04.07.2019
First-principles-based calculations of caloric effects in ferroelectrics and multiferroics
C. Ederer
ETH Zürich, Switzerland

11.07.2019
Deformation and defects in minerals: insights from atomic-scale simulations
P. Hirel
Université de Lille, Villeneuve d'Ascq, France

04.09.2019
FE2TI – Combining computational homogenization and domain decomposition methods for the simulation of dual-phase steel
A. Klawonn, M. Lanser
Universität zu Köln, Germany

11.09.2019
Molecular simulations you can trust and reproduce: the OpenKIM framework
R. S. Elliott
University of Minnesota, Minneapolis, USA

11.09.2019
Non-monotonic rheology of a magnetic liquid crystal mixture in an external field
N. Hamidi Siboni
TU Berlin, Germany

18.09.2019
High quality phase diagrams – a roadmap for a successful casting processing
P. Presoly
Montanuniversität Leoben, Austria

17.10.2019
Describing the charged defect redistribution in a ferroelectric domain structure with the Landau-Ginzburg-Devonshire theory
I. Vorotiahin
TU Darmstadt, Germany

13.11.2019
Interatomic potentials from permutation-invariant polynomials
C. Ortner
University of Warwick, Coventry, UK

15.11.2019
A phase-based, physics-informed framework for materials AI
R. Otis
Pennsylvania State University, State College, USA

02.12.2019
A multi-scale numerical model for crack propagation in a matrix with inclusions
T. Karakasidis
University of Thessaly, Volos, Greece

07.01.2020
Material-oriented ultra-precision machining: case studies of polycrystalline metal and reaction-bonded ceramic
J. Zhang
Central South University, Changsha, China

13.01.2020
High-dimensional neural network potentials for atomistic simulations
J. Behler
Georg-August-Universität Göttingen, Germany

05.03.2020
New permanent magnet phases from computational design
H. C. Herper
Uppsala University, Sweden

ICAMS

Teaching

19. Teaching

► MSS lecture courses summer term 2019

R. Drautz
Data-driven materials science

T. Hammerschmidt, R. Janisch
Interfaces and surfaces

G. Sutmann
Introduction to parallel- & scientific computing

I. Roslyakova
Material informatics with R

M. Mrovec
Mathematics for materials modelling

A. Hartmaier
Microstructure and mechanical properties

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

R. Drautz
Quantum mechanics in materials science

► MSS lecture courses winter term 2019/20

J. Rogal
Advanced atomistic simulation methods

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

R. Drautz
Atomistic simulation methods

R. Janisch, S. Brinckmann
Assessment and description of material properties

A. Hartmaier, N. Vajragupta
Computational fracture mechanics

I. Steinbach
Continuum methods in materials science

R. Drautz, A. Grünebohm, M. Piacenza
Documenting and communicating science

G. Eggeler
Elements of microstructure

T. Li
Introduction to 3-dimensional materials characterization techniques

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

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

F. Pöhl
Materials processing

R. Janisch
Multiscale mechanics of materials

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

I. Steinbach
Solidification processing

I. Roslyakova
Statistical methods in data analysis and design of experiments

F. Varnik
Statistical physics and thermodynamics

T. Hammerschmidt, M. Mrovec
Theory and application of bond order potentials

► Block course on modelling – University of Oxford, 19.01.2020 - 25.01.2020

R. Drautz
Introduction to modelling in materials science

► Block course – Harbin Institute of Technology. 15.-18. 07. 2019

A. Hartmaier
Materials-oriented (nano-) manufacturing

► MSS lecture courses summer term 2020 (online classes)

T. Hammerschmidt, R. Janisch
Atomistic aspects of materials properties

R. Drautz
Data-driven materials science

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

T. Hammerschmidt, G. Sutmann
Introduction to parallel- and scientific computing

I. Roslyakova
Material informatics with R

M. Mrovec
Mathematics for materials modelling

A. Hartmaier
Microstructure and mechanical properties

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

A. Grünebohm, I. Eremin
Physics of complex phase transitions in solids

R. Drautz
Quantum mechanics in materials science

► MSS lecture courses winter term 2020/21 (online classes)

A. Grünebohm, M. Mrovec
Advanced atomistic simulation methods

A. Hartmaier, R. Janisch
Assessment and description of material properties

R. Drautz
Atomistic simulation methods

N. Vajragupta
Computational fracture mechanics

I. Steinbach
Continuum methods in materials science

A. Grünebohm, M. Piacenza
Documenting and communicating science

G. Eggeler
Elements of microstructure

T. Li
Introduction to 3-dimensional materials characterization techniques

T. Hickel
Introduction to quantum mechanics

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

M. Stricker
Materials informatics

F. Pöhl
Materials processing

A. Hartmaier
Multiscale mechanics of materials

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

I. Steinbach
Solidification processing

F. Varnik
Statistical physics and thermodynamics

T. Hammerschmidt, M. Mrovec
Theory and application of bond order potentials

► ICAMS Graduate School

Part I: Atomistic Modelling and Simulation, block course from 01.-02.10.2020

The second block course (The phase-field approach) will take place from 13.04.-14.04.2021.

The third block course (Micromechanical and macroscopic modelling) will take place from 01.09.-02.09.2021.

► Block course – Harbin Institute of Technology. 07.-17.07.2020

A. Hartmaier
Materials-oriented (nano-) manufacturing

► Block course on modelling – University of Oxford, 16.11.2020 - 20.11.2020

R. Drautz
Introduction materials modelling

► SurMat – Simulation and modeling, 05.10.-08.10.2020

J. Neugebauer
Electronic structure methods

R. Drautz
Atomistic simulations

I. Steinbach
Mesoscale simulations

A. Hartmaier
Continuum methods

ICAMS

ICAMS Members 2019 and 2020

20. ICAMS Members 2019 and 2020

▸ Staff at ICAMS

About 70-80 researchers, including PhD students, work at ICAMS; about five administrative staff and two technicians support the institute.

Figure 20.1 shows the development of ICAMS staff numbers through the past eleven years. By the end of 2010 about 57 people were working at ICAMS. From 2011 to 2014 this number increased and by the end of 2014 almost 90 people worked at ICAMS. Since the end of the start-up funding in 2013, staff numbers decreased due to a smaller number of industry projects. Since 2017, the number of employees has leveled off at around 80. The majority of ICAMS scientists hold a degree in engineering and materials science, followed by degrees in physics, mathematics or computer science and chemistry (*Fig. 20.2*). This educational diversity of our research staff provides the basis for ICAMS' interdisciplinary research.

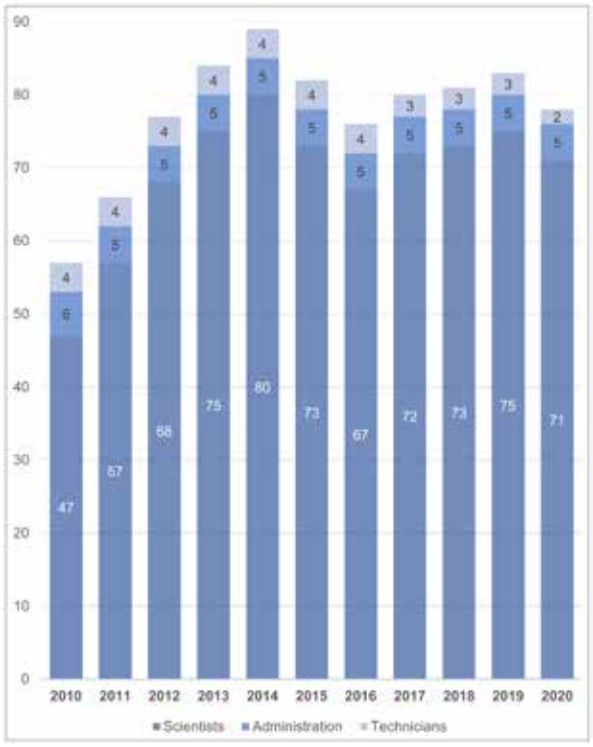


Fig. 20.1: Development of ICAMS staff from 2010 to 2020.

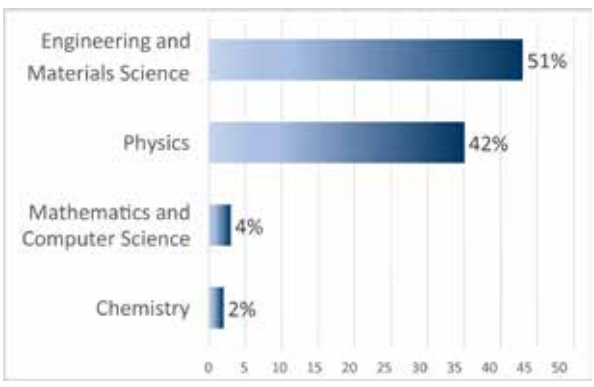
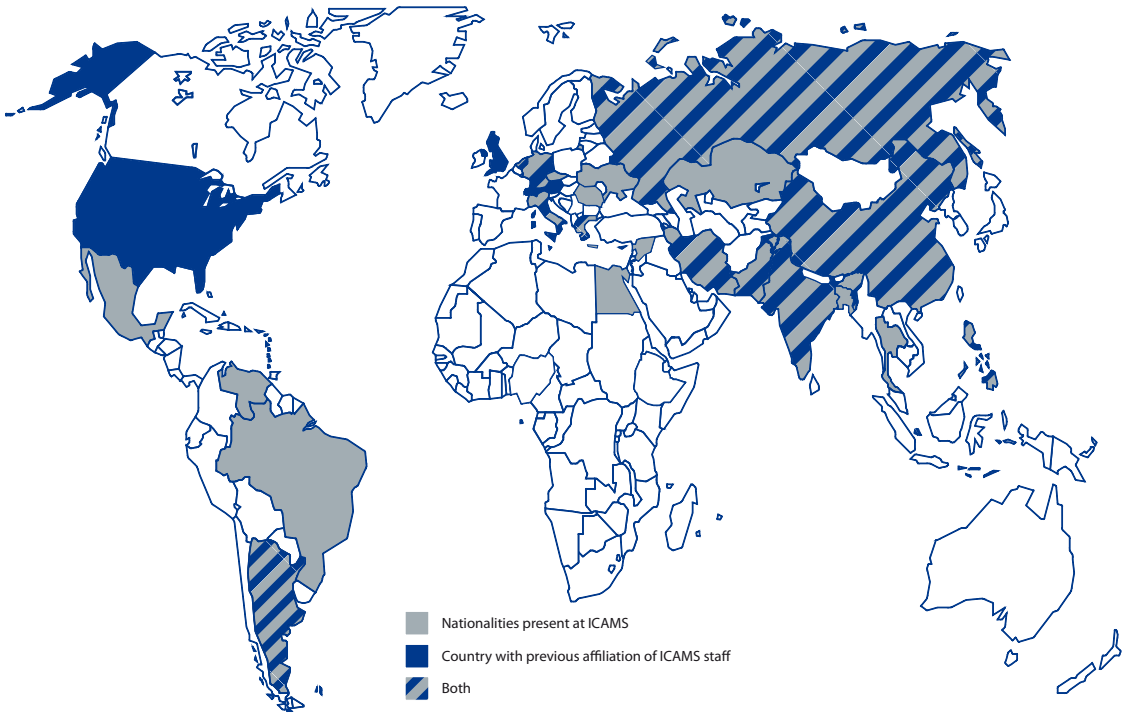


Fig. 20.2: Breakdown of first degree of ICAMS researchers in 2019/2020.

In 2019 and 2020 researchers from 23 different countries were working at ICAMS (see grey areas in *Fig. 20.3*). 34% of the ICAMS staff is of German and 66% of foreign nationality. For ICAMS, it is of vital importance to attract talented scientists from leading research institutions worldwide.

Figure 20.3 gives an overview of the countries and institutions of origin of the current ICAMS researchers. 13 of the 39 institutions are located in Germany, 14 in other EU countries and 12 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

Argentina
National University of General San Martin

Austria
Technical University of Vienna

China
Northwestern Polytechnical Univ., Xi'an Shaanxi
Tianjin University, Tianjin

France
FEMTO-ST, Besancon
LEM-ONERA-CNRS, Chatillion
CEA Grenoble
CNRS, Paris

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

Greece
University of Ioannina

India
Indian Institute of Science, Karnataka

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

Italy
NNL of CNR-INFM, Lecce
Politecnico di Milano
University of Trento
University of Trieste

The Netherlands
University of Amsterdam
TU Delft

Pakistan
Ghulam Ishaq Khan Institute of Engineering

Philippines
De La Salle University, Manila

Russia
Kazan Federal University
JIHT Moskow

Switzerland
EPFL, Lausanne

United Kingdom
University of Oxford

USA
University of Rochester (NY)

Fig. 20.3: 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.

Dr. Katrin Abrahams
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation
(at ICAMS until 15.07.2020)

Dr. Masud Alam
Postdoctoral Researcher
Micromechanical and Macroscopic Modelling

M.A. Pia Aleithe
MRD Coordinator

M.Sc. Muhammad Adil Ali
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation

Dr. Waseem Amin
Doctoral Candidate
Micromechanical and Macroscopic Modelling
(at ICAMS until 31.12.2020)

M.Sc. Abril Azócar Guzmán
Doctoral Candidate
Micromechanical and Macroscopic Modelling

Prof. Dr. Daniel Balzani
Advanced Study Group Leader
Continuum Mechanics

Dr. Abhishek Biswas
Postdoctoral Researcher
Micromechanical and Macroscopic Modelling

Prof. Dr.-Ing. Wolfgang Bleck
Advanced Study Group Leader
Processing and Characterization

Dr. Anton Bochkarev
Postdoctoral Researcher
Atomistic Modelling and Simulation

M.Sc. Marian Bruns
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation

Niklas Caesar
IT System Administration
IT Adminstration
(at ICAMS until 31.01.2019)

M.Sc. Ashish Chauniyal
Doctoral Candidate
Micromechanical and Macroscopic Modelling

Dr. Grisell Díaz Leines
Postdoctoral Researcher
Atomistic Modelling and Simulation
(at ICAMS until 31.08.2020)

M.Sc. Aris Dimou
Doctoral Candidate
Scale-Bridging Simulation of Functional Composites

Dr. Sergiy V. Divinski
Advanced Study Group Leader
Diffusion and Microstructure Analysis

Prof. Dr. Ralf Drautz
Director
Atomistic Modelling and Simulation

Prof. Dr.-Ing. Gunther Eggeler
Advanced Study Group Leader
Input Data and Validation

M.Sc. Aleksei Egorov
Doctoral Candidate
Atomistic Modelling and Simulation

Dr.-Ing. Jenni Kristin Engels
Doctoral Candidate
Micromechanical and Macroscopic Modelling
(at ICAMS until 04.06.2019)

Dr. Alberto Ferrari
Doctoral Candidate
Atomistic Modelling and Simulation
(at ICAMS until 31.08.2019)

Dr. Mariano Daniel Forti
Postdoctoral Researcher
Atomistic Modelling and Simulation

Prof. Dr.-Ing. Jan Frenzel
Advanced Study Group Leader
Input Data and Validation

Dr. Suzana G. Fries
Research Group Leader
Scale-Bridging Thermodynamic and Kinetic Simulation
(at ICAMS until 30.06.2019)

Dr.-Ing. Siwen Gao
Postdoctoral Researcher
Micromechanical and Macroscopic Modelling
(at ICAMS until 31.12.2019)

Dr. Johannes Viktor Görler
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M.Sc. Haifeng Wang
Doctoral Candidate
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Dr. Ning Wang
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Prof. Dr. Gerhard Wilde
Advanced Study Group Leader
Diffusion and Microstructure Analysis

M.Sc. Hui Cheng Xia
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M.Sc. Setareh Zomorodpoosh
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation

IAMS

Guests and Visitors

21. Guests and Visitors

Most of the guests and seminar speakers in 2020 visited ICAMS virtually.

Anthony Akinwale
Department of Materials
University of Oxford
Oxford, UK
08.07.2019 - 31.08.2019

Juan M. Anduqía Restrepo
Departamento Ingeniería Mecnica y Mecatrónica
Universidad Nacional de Colombia (UNAL)
Bogotá, Colombia
01.02.2019 - 01.08.2019

Dr. Chandler A. Becker
Office of Data and Informatics, Material Measurement Laboratory
US National Institute of Standards and Technology
Gaithersburg, USA
10.04.2019

Prof. Dr. Jörg Behler
Institut für Physikalische Chemie
Georg-August-Universität Göttingen
Göttingen, Germany
13.01.2020

Prof. Dr. Malte Behrens
Materials Chemistry of Catalysis
Universität Duisburg-Essen
Duisburg, Germany
06.06.2019

Dr.-Ing. Simon Bonk
Department of applied materials physics
KIT Karlsruhe Institute of Technology
Karlsruhe, Germany
18.03.2019 - 22.03.2019

Harry Chapman
Department of Materials Science
University of Oxford
Oxford, UK
04.07.2019 - 31.08.2019

Dr. Dmitry Chigrin
Leibniz-Institut für Interaktive Materialien
RWTH Aachen
Aachen, Germany
29.10.2020

Dr. Jan Willem Coenen
Forschungszentrum Jülich
Jülich, Germany
13.05.2019

Prof. Diederik Depla
Solid state sciences department
Ghent University
Ghent, Belgium
10.01.2019

Prof. Dr. David Dye
Imperial College London
London, UK
09.05.2019

Prof. Dr. Claude Ederer
Department of Materials Theory
ETH Zürich
Zürich, Switzerland
02.07.2019 - 05.07.2019

Diema El-Lahib
Ruhr-Universität Bochum
Bochum, Germany
01.12.2020 - 30.04.2021

Prof. Dr. Ryan S. Elliott
University of Minnesota
Minneapolis, USA
10.09.2019 - 13.09.2019

Prof. Dr. Michael Finnis
Department of Materials
Imperial College London
London, UK
03.06.2019 - 30.06.2019

Dr. Benjamin Geisler
Computational Materials Physics
Universität Duisburg-Essen
Duisburg, Germany
09.07.2020

Prof. Dr. Nina Gunkelmann
Institute of Applied Mechanics
TU Clausthal
Clausthal-Zellerfeld, Germany
12.12.2019

Dr. Nima Hamidi Siboni
Institute of Theoretical Physics
TU Berlin
Berlin, Germany
11.09.2019

Dr. Heike C. Herper
Uppsala University
Uppsala, Sweden
05.03.2020

Dr. Ralf Hielscher
Applied Functional Analysis
TU Chemnitz
Chemnitz, Germany
03.06.2019

Prof. Dr. Pierre Hirel
Unité Matériaux et Transformations
Université de Lille
Villeneuve d'Ascq, France
11.07.2019

Hossein Jafarzadeh
Sharif University of Technology
Teheran, Iran
19.06.2019 - 28.06.2019

Jan Janßen
Department Computational Materials Design
Max-Planck-Institut für Eisenforschung
Düsseldorf, Germany
06.10.2020

Prof. Dr. Surya R. Kalidindi
Georgia Institute of Technology, Georgia Tech
Atlanta, USA
28.01.2020 - 01.02.2020

Prof. Dr. Theodore Karakasidis
University of Thessaly
Volos, Greece
01.12.2019 - 07.12.2019

Prof. Dr. Markus Kästner
Institute of Solid Mechanics
TU-Dresden
Dresden, Germany
24.01.2019

Dr. Ursula R. Kattner
Materials Science and Engineering Division
National Institute of Standards and Technology
Gaithersburg, USA
25.05.2019 - 31.05.2019

Dr. Ruben Khachaturyan
Institute of Materals Science – Materials Modelling Division
TU Darmstadt
Darmstadt, Germany
04.06.2019

Prof. Dr. Axel Klawonn
Cologne University
Köln, Germany
04.09.2019

Prof. Dr. Manfred Kohl
Institute of Microstructure Technology
Karlsruhe Institute of Technology (KIT)
Eggenstein-Leopoldshafen, Germany
23.01.2020

Dr. Timm Krüger
Multiscale Thermofluids
University of Edinburgh
Edinburgh, UK
21.11.2019

Dorota Kubacka
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Erlangen, Germany
25.03.2019 - 29.03.2019

Prof. Ing. Pavel Lejcek
Institute of Physics
Academy of Sciences
Prague, Czech Republic
30.01.2019 - 01.02.2019

Dr. Hao Lyu
Material Science and Engineering
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Erlangen, Germany
11.02.2019 - 15.02.2019

Daria Malakhova
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Kazan, Russia
01.03.2019 - 31.05.2019

Dr. Francesco Maresca
University of Groningen
Groningen, The Netherlands
29.05.2019

Prof. Dr. Svea Mayer
Werkstoffwissenschaft
Montanuniversität Leoben
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04.07.2019

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17.05.2019

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11.11.2019 - 19.11.2019

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03.04.2019 - 02.06.2019

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03.06.2019 - 08.06.2019

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23.05.2019

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16.10.2019 - 20.10.2019

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22.11.2019 - 22.12.2019

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