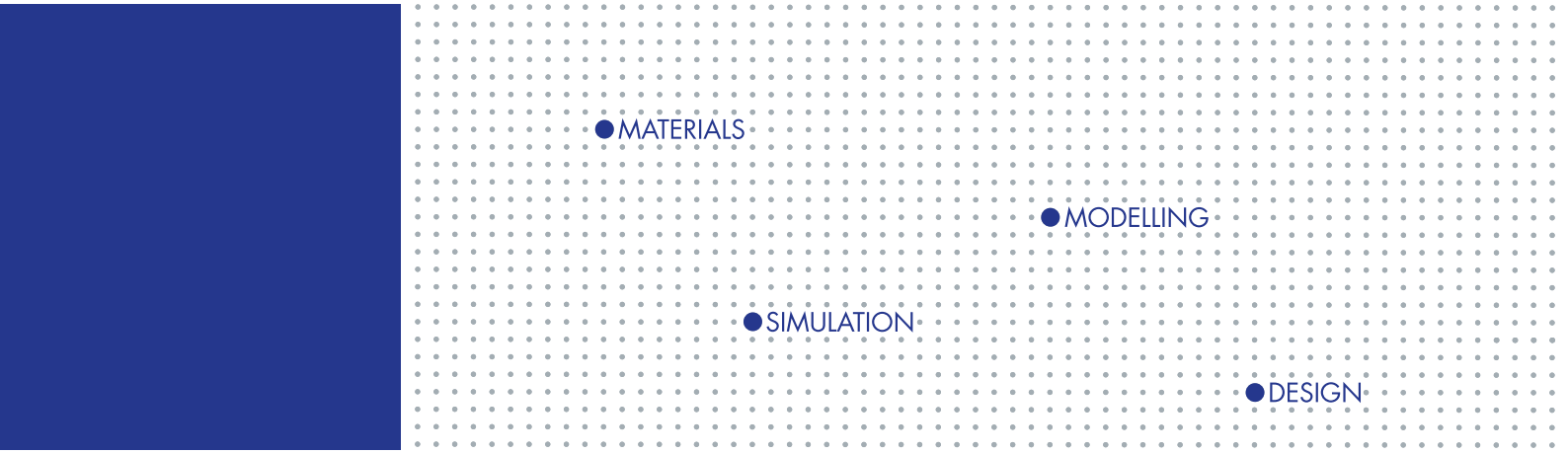
Scientific Report 2023 and 2024



ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Contents

ICAMS

Scientific Report 2023 and 2024

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1. Preface

The scientific field of advanced materials modelling has rapidly evolved in the past years. The main driving factor was the increased availability and applicability of research data and data-driven methods in materials science. Furthermore, the general availability of large language models is just starting to reshape our field. ICAMS adopted these methods at an early stage in its research and teaching activities and thus made significant contributions to their further development.

This report summarizes our research and teaching activities in the past two years. New research projects started, and we restructured the curriculum of our Master's course, one of the most successful international programs at Ruhr-Universität Bochum.

We want to thank all our collaborators, partners and friends from all over the world, the funding agencies, mainly the Deutsche Forschungsgemeinschaft (DFG), Ruhr-Universität Bochum and, last but not least, our staff members and students for contributing to ICAMS' continued success.

We hope you enjoy reading.

Alexander Hartmaier
Managing Director

Silvana Botti

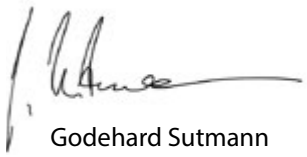
Ralf Drautz

Anna Grünebohm

Miguel Marques

Markus Stricker

Ingo Steinbach



Godehard Sutmann

ICAMS

ICAMS in 2023 and 2024

2. ICAMS in 2023 and 2024

ICAMS is an internationally visible, leading scientific competence centre in the field of advanced computational materials science. Its interdisciplinary and multidisciplinary research, teaching, and qualification program of the next generation of materials scientists focuses on the relationship between the structure and the properties of materials.

ICAMS' problem-driven research brings forth solutions across the relevant length and time scales in the form of novel methods, including software, data science approaches and the discovery of new materials to the benefit of science, industry, and society.

In its teaching and qualification programs, ICAMS covers the breadth of modern multidisciplinary materials science and simulation. In addition, it is involved in scientific training by teaching the latest methodological skills. As a theory and tool provider, we drive and inspire the entire field of computational materials science.

The rapid development of Large Language Models (LLM) makes powerful artificial intelligence (AI) tools broadly available, which, among many societal aspects, also has a profound impact on research and teaching. LLMs can be used as supporting tools for writing of scholarly texts and computer code, or to setup parametric studies or even entire workflows. In its current research activities, ICAMS explores the possibilities of using LLMs for data extraction and curation. In the future, they could provide natural language interfaces to simulation tools, making them available also to non-experts. Students already increasingly rely on LLMs for their literature surveys, for providing explanations to scientific concepts touched in lectures, or even to find solutions to given tasks. As any new technology, LLMs hold promises and risks, and we need to find a proper way to include them in a meaningful way into our research and teaching. Recent progress in machine-learning interatomic potentials have led to the development of foundation models capable of simulating in principle any material, molecule or combination thereof. The joint development of graph neural networks, in particular the graph atomic cluster expansion (GRACE), together with the Alexandria database, places ICAMS at the forefront of this revolution in atomistic simulation.

In the past two years, ICAMS researchers have been able to raise over € 9.5 million in research funding. Most of the projects were funded by the Deutsche

Forschungsgemeinschaft (DFG). The three largest individual projects are, however, the EU-funded "Hard work, plastic flow: a data-centric approach to dislocation-based plasticity (DISCO-DATA)" by Markus Stricker, the BMBF funded "Digital material analysis along the entire value chain (DiStEL)" by Ingo Steinbach and "Quantum geometry in 3D materials" by Miguel Marques, which is funded by the Tschira Foundation.

As proposed by the Advisory Board, the concept of the Advanced Study Groups was replaced by the ICAMS Fellows. ICAMS Fellows are close and long-term collaborators from other institutions that contribute to ICAMS research, teaching, or the organisation of joint events. The first ICAMS Fellows are:

- **Prof. Dr. Sergiy Divinskiy**,
  Institut für Materialphysik, Universität Münster
- **Prof. Dr. Gunther Eggeler**,
  Institute for Materials, Ruhr-Universität Bochum
- **Prof. Dr. Jan Frenzel,**
  Institute for Materials, Ruhr-Universität Bochum
- **Dr. Tilmann Hickel,**
  BAM Berlin, and Max Planck Institute for Sustainable Materials, Düsseldorf
- **Prof. Dr. Pierre Hirel,**
  Unité Matériaux et Transformations, Université de Lille
- **Prof. Dr Jörg Neugebauer,**
  Max Planck Institute for Sustainable Materials, Düsseldorf
- **Prof. Dr. Thomas Niendorf,**
  Institut für Werkstofftechnik, Universität Kassel

Teaching

Bachelor program in Materials Science

The bachelor's course "Materialwissenschaft" (Materials Science) is starting its third year. The number of applicants is falling short of expectations; the trend of declining student numbers can be observed nationwide in materials science and engineering courses and, in fact, in most of the STEM subjects. Together with colleagues from the Institute of Materials, we started a new series of summer schools for middle and high-school students as one activity to increase the visibility of the BSc programme. Besides this long-term activity, it is planned to visit more schools and to advertise this course together with Mechanical Engineering. The situation needs to be monitored closely, and measures, such as changing the curriculum to English to attract more international students are being discussed.

Master's course Materials Science and Simulation (MSS)

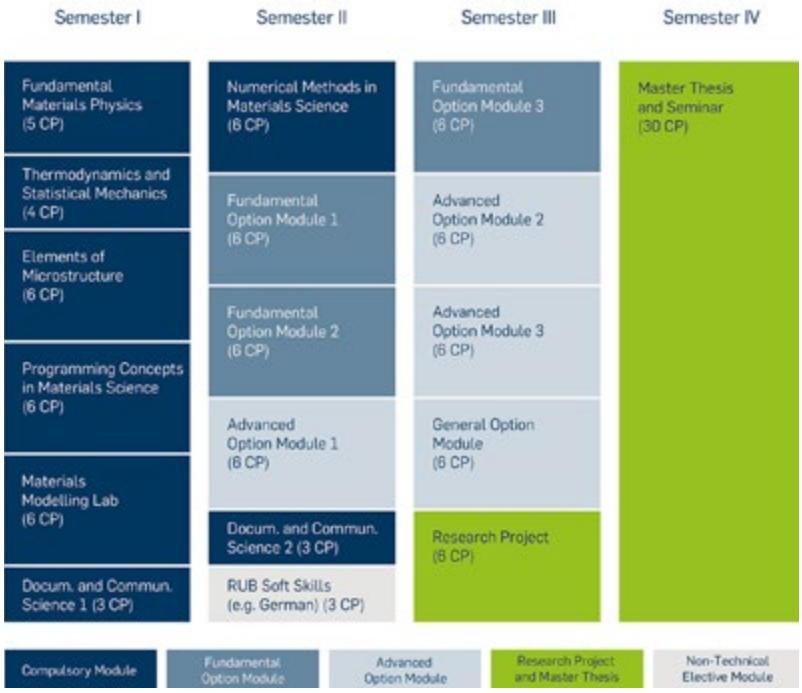


Fig. 2.1: New curriculum of the master's program Materials Science and Simulation (MSS).

After its excellent evaluation by AQAS e.V. and the Stiftung Akkreditierungsrat in 2023, our international master's program has been re-certified.

After thorough internal discussions we decided to apply some major changes to its curriculum and examination regulations. The primary motivations for revising the program are attracting more talented students from diverse backgrounds, allowing for earlier specialization, and incorporating new topics reflecting changes in the scientific landscape. These changes are also mirrored in the expertise brought by our new professors, who are leaders in their respective fields.

The Materials Modelling Lab, a hands-on course of the first semester, provides our students with a basic overview of modern materials simulation methods, allowing them to pick a choice for their individual specialization along our fundamental and advanced option modules in the subsequent semesters.

New modules, e.g. from the field of materials informatics and data science add to the modern character of our course.

In 2023 we received more than 1350, and in 2024, almost 1650 applications for our master's programme "Materials Science and Simulation". Altogether 59 students eventually took up their studies in the last two years. 14 master's students successfully graduated in 2023 and 17 in 2024.

Fortunately, the trend in this international degree program is, contrary to the general development, moving into a very positive direction, and student numbers are increasing.

Fig. 2.2: MSS fresher's day 2024.

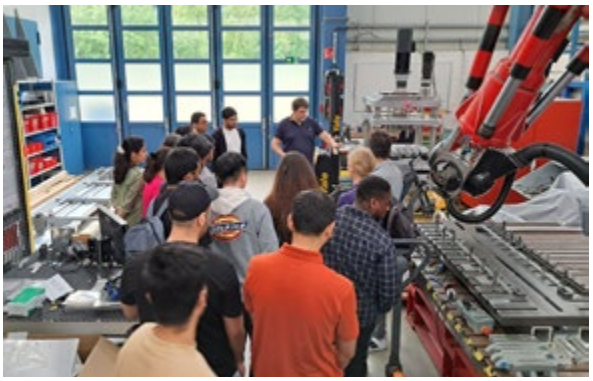


Fig. 2.3: MSS excursions to Berlin 2023 (upper left picture) and Hamburg 2024 (lower left).

Fig. 2.4: Fireplace talk 2024 (upper right pictue), visit to DLR Cologne 2023 (lower right).

After the pandemic years, ICAMS has resumed regular excursions to bring MSS students into contact with companies in Germany. The 2023 excursion went to Berlin, Salzgitter and Wolfsburg, the 2024 excursion went to Hamburg with visits to the IWT Bremen, the Helmholtz-Zentrum Hereon, Geesthacht, and DESY Hamburg. Visits to regional companies in the Ruhr area are planned for the future.

On the students' own initiative, a guided tour took place at DLR Cologne in 2023, in which doctoral students also took part.

Regular “fireplace talks”, at which ICAMS graduates present their work experience after graduation and introduce career prospects in a relaxed and informal atmosphere, further facilitate interactions between ICAMS students and industry. In 2024, two fireplace talks, which were held in presence again, hosted Michele Matsuo from Otto Fuchs KG, Meinerzhagen and Martin Boeff from Siemens Energy, Gelsenkirchen, as well as Ari Harjunmaa from Accenture Song Content, Stuttgart.

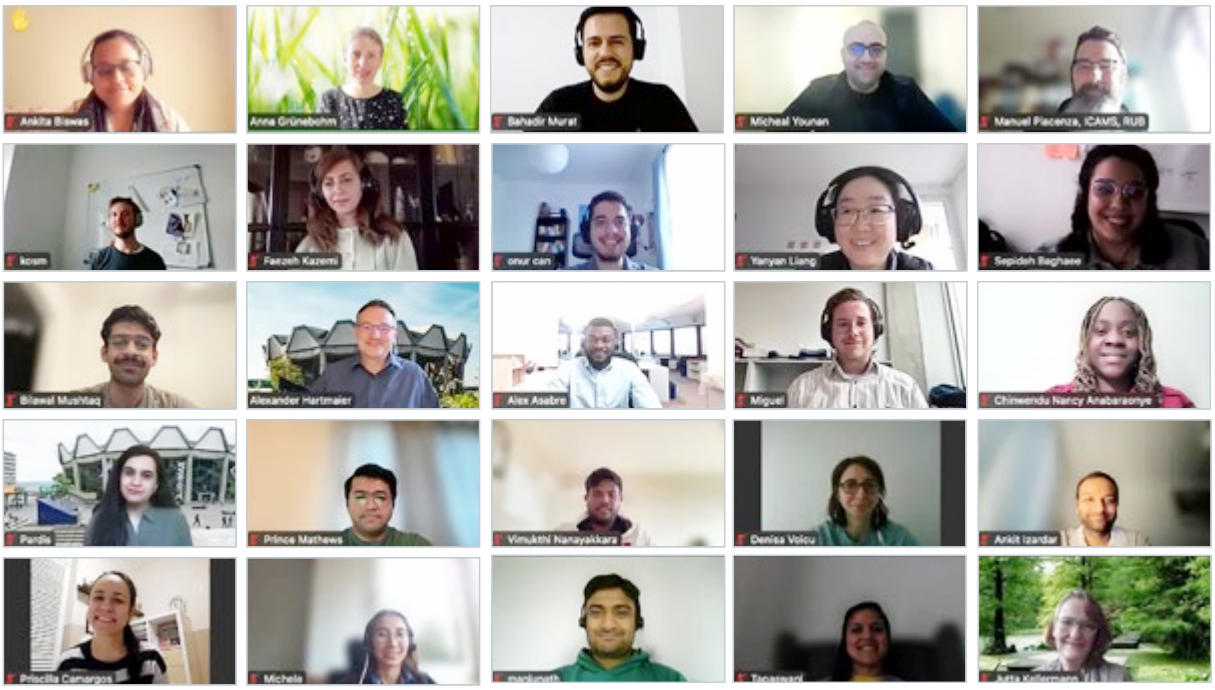


Fig. 2.5: MSS Alumni-meeting (online).

The ICAMS Master Fair took place twice in 2023, namely in January and November. The ICAMS professors gave an overview of the research fields of their departments and presented master thesis topics. The last ICAMS Master Fair took place in January 2025.

MSS Alumni-Meeting 04. 04. 2024
In preparation for the Advanced Discussions dedicated to ICAMS alumni in fall 2024, an MSS alumni meeting was held online in spring 2024. Former students gave valuable feedback on how the skills they acquired at ICAMS can be used in their current work routine. They also gave tips on which skills can be useful beyond that.

Rutopia discussions

The Rutopia panel discussions started in summer 2023 and are open to all PhD and master students as well as researchers at ICAMS / Institute for Materials and related fields. Anna Grünebohm and Tong Li moderate the new format. The individual events were focused on the topics "What is a PhD about?", "Is ChatGPT good for my research?" and "Share your stories: Survive the German academic system with diverse backgrounds".

Max Planck Research School SusMet

The Max Planck Research School on Sustainable Metallurgy started in 2022. It offers 37 PhD positions and is coordinated at the MPIE in Düsseldorf. ICAMS is one of the project partners. Its research focuses on the exploration of carbon-free sustainable metallurgy, employing hydrogen as reducing agent, direct electroreduction (electrolysis) and plasma synthesis.

Workshops and Conferences

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

At the 2023 Advanced Discussions: Application of machine learning and data science for scale-bridging materials simulation, participants from academia and industry presented and discussed recent developments. The 2024 edition of the Advanced Discussions was dedicated to our ICAMS Alumni: "From ICAMS into the world: Careers in academia and industry".

The 2023 Materials Chain International Conference was titled "Materials Science Meets Artificial Intelligence – Advancements in Research and Innovation". International speakers from various disciplines discussed current developments and open questions in data-driven materials science, from atomistic to microstructure descriptions and structure-property relationships as well as in research data management.

The 2024 Materials Chain International Conference was focused on Inorganic Functional Materials: Developments and Applications for Advanced Technologies and brought together researchers, scientists and industry professionals to explore the latest advancements and applications of inorganic functional materials.

Fig. 2. 6: ICAMS Advanced Discussion 2023 (group picture and picture taken at the poster session).

Fig. 2.7: ICAMS retreat 2024.

Fig. 2.8: Kimia NouraniNiaki and Murali Uddagiri won a poster prize at the International Phase-Field Modelling Symposium in Hangzhou, China (left). Humboldt awardee Prof. Dr. Yonggang Huang visited ICAMS in October 2024 (photo Tim Kramer, RUB).

Other conferences and events with significant contributions to their organization from ICAMS were:

2023

- AI MSE 2023, Hybrid Conference, Saarbrücken
- DGM Working Group Microstructural Mechanics, TU Berlin

2024

- MRD Industry Day 2024, RUB, Bochum
- The 5th International Symposium on Phase-Field Modelling in Materials Science, Hangzhou, China
- CECAM Flagship Workshop Machine Learning Potentials: From Interfaces to Solution

Prof. Dr. Yonggang Huang of Northwestern University in USA has won the Humboldt Research Award upon nomination by Alexander Hartmaier. He already visited ICAMS and will spend more time in 2025 here to collaborate on fatigue and lifetime modeling of metallic interconnects in flexible electronics.

Summer School Materialwissenschaft

The new "Summer School Materialwissenschaft" is intended to give students from the 10th class the opportunity to get a first insight into materials science in exciting projects and experiments. Organized by ICAMS and the Institute for Materials, Anna Grünebohm and Markus Stricker, among others, are responsible for the project, which started in summer 2023. As an equal-opportunity measure, the summer school is offered every other year for female (f/d) attendants only.

Outing

The 2023 ICAMS outing took the participants to Bottrop. A hike led up to the landmark tetrahedron, which most participants climbed and which offered a great view over the Ruhr area. Afterwards, a visit to the former Prosper Haniel mine site offered lots of fun with detective games in a historically designed escape room setting, where the aim was to solve puzzles in teams.

In 2024, a shared picnic with barbecues and lawn games on the premises of RUB offered everyone the opportunity to spend some time together and get to know each other better. Master's and Bachelor's students also took part.

Fig. 2.9: Summer School Materialwissenschaft 2023 and 2024.

Fig. 2.10: ICAMS outings 2023 and 2024.

ICAMS

Organisation of ICAMS

3. Organisation of ICAMS

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

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

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Prof. Dr. Fathollah Varnik	Department Scale-Bridging Thermodynamic and Kinetic Simulation

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ICAMS

Department Atomistic Modelling and Simulation AMS

4. Department Atomistic Modelling and Simulation

Prof. Dr. Ralf Drautz

▸ Research

The Department for Atomistic Modelling and Simulation has two main objectives:

1. The development of efficient interatomic potentials.
2. The application of the interatomic potentials to understand, predict and design materials.

In particular, the Department has developed the Atomic Cluster Expansion (ACE) and its extension to include graphs, the Graph Atomic Cluster Expansion (GRACE). ACE and GRACE are among the fastest and most accurate machine learning interatomic potentials.

The Department provides the complete development stack required for ACE and GRACE, including basic theory and derivation, implementation in efficient software for large scale simulations, software for training of ACE and GRACE models and tools for validation and application. These developments are supported by automated high-throughput workflows for generating density functional training data.

Recent extensions of ACE and GRACE enable incorporation of charge transfer, simulation of magnetic materials and prediction of vectorial, tensorial and spectral properties. Effective embedding of chemical space allows us to train leading foundation models that cover the complete periodic table.

▸ Structure

The Department has three research groups:

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

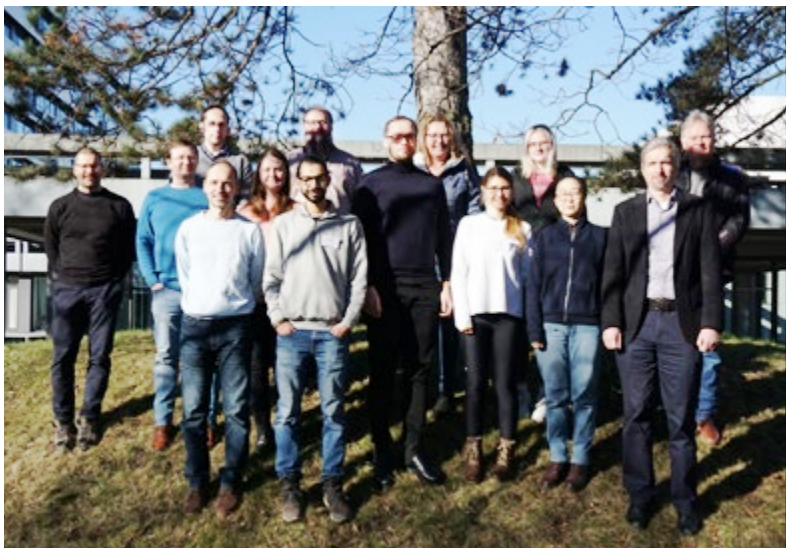

Fig. 4.1: Cover art of two recent publication in the Journal of Chemical Theory and Computation. Right: Efficient Parametrization of Transferable Atomic Cluster Expansion for Water, E. Ibrahim, Y. Lysogorskiy, and R. Drautz, Journal of Chemical Theory and Computation 2024, 20, 24, 11049-11057, Left: Atomic Cluster Expansion for Quantum-Accurate Large-Scale Simulations of Carbon, M. Qamar, M. Mrovec, Y. Lysogorskiy, A. Bochkarev, and R. Drautz, Journal of Chemical Theory and Computation 2023, 19, 15, 5151-5167.

AMS

4.1. Data-Driven Methods for Atomistic Simulations

Group leader:
Dr. Yury Lysogorskiy

Group members:
Dr. Anton Bochkarev
Eslam Ibrahim

▸ Research

The research group focuses on the development and application of Atomic Cluster Expansion (ACE) and its extension, Graph Atomic Cluster Expansion (GRACE) – a new class of machine learning interatomic potentials (MLIPs) with a formally complete basis set that extends ACE to incorporate semilocal interactions.

Our work spans the entire ACE/GRACE model development pipeline, including reference data generation, parameterization, and validation, as well as their integration into high-performance simulation codes such as LAMMPS.

Recently, our efforts have been dedicated to the parameterization of universal MLIPs-models that span the entire periodic table, enabling out-of-the-box simulations of diverse material systems with decent accuracy. These universal MLIPs also serve as foundation models, accelerating the development of more accurate, material-specific MLIPs while significantly reducing the need for large training datasets.

▸ Competences

- Density functional theory and molecular dynamics simulations
- Atomic Cluster Expansion (ACE) / Graph Atomic cluster expansion (GRACE): method development, parameterization and validation
- Universal machine learning interatomic potentials (uMLIP): development interatomic potentials for complete periodic table.

Active learning strategies for atomic cluster expansion models

Machine learning potentials can fail drastically when applied outside their training data domain. To ensure reliable simulations with MLIPs, it is crucial to employ an uncertainty indication mechanism that signals the reliability of model predictions. We demonstrate that using the D-optimality criterion for ACE models reliably identifies extrapolation events with an extrapolation grade, facilitating active learning and exploration of training configurations. This approach accelerates and automates the construction and parameterization of reliable, transferable MLIPs.

Y. Lysogorskiy, A. Bochkarev, M. Mrovec, and R. Drautz, Active learning strategies for atomic cluster expansion models,
Physical Review Materials, 7(4), 043801, 2023

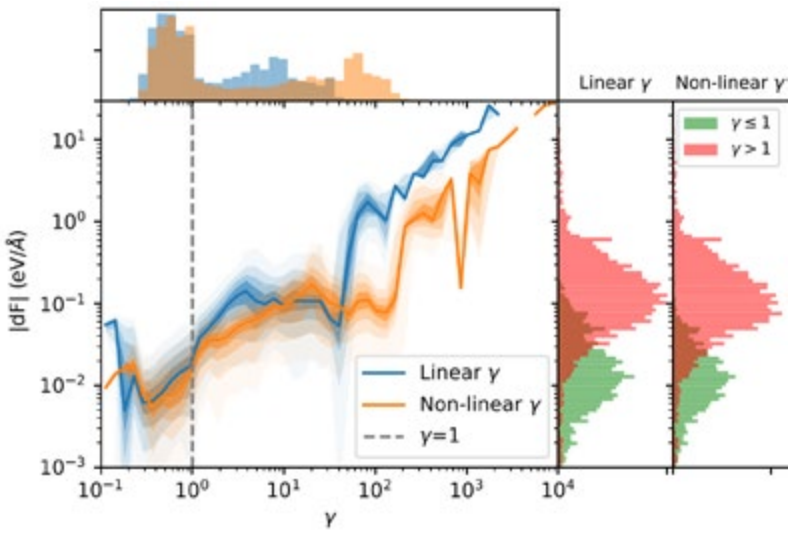

Fig. 4.2: Analysis of force errors for the linear and nonlinear extrapolation grades for the Cu-III dataset. Error distribution for interpolative (green) and extrapolativew (red) configurations.

From electrons to phase diagrams with machine learning potentials using pyiron based automated workflows

In this work, we present a standardized and automated workflow for developing Atomic Cluster Expansion (ACE) interatomic potentials within the pyiron framework. Our approach streamlines the entire development cycle, from generating systematic DFT databases to fitting ACE models and validating their performance across diverse material properties. By employing active learning and uncertainty quantification, we enhance the transferability and reliability of ACE-based potentials. As a case study, we demonstrate the computation of an Al-Li phase diagram, showcasing the framework's capability to efficiently construct accurate and scalable MLIPs for complex material system.

S. Menon, Y. Lysogorskiy, A. L. Knoll, N. Leimeroth, M. Poul, M. Qamar, and J. Neugebauer,
From electrons to phase diagrams with machine learning potentials using pyiron based automated workflows,
npj Computational Materials, 10(1), 261, 2024

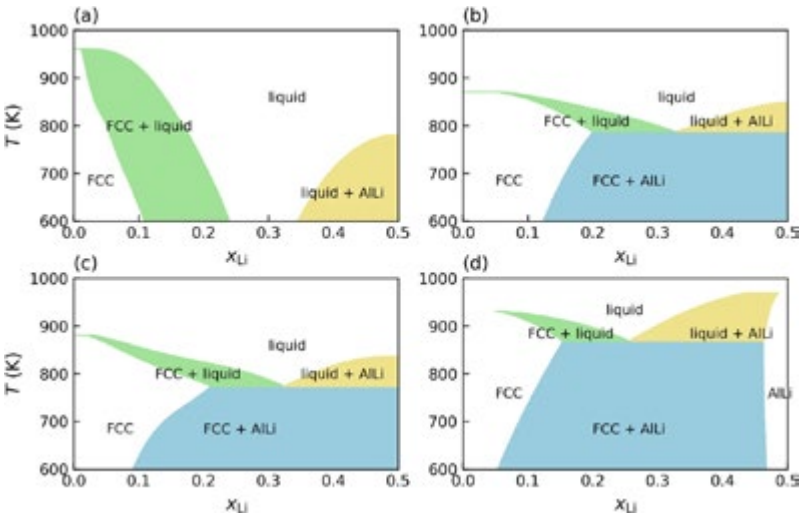

Fig. 4.3: Phase diagram of Al-Li up to xLi = 0.5 computed with ACE interatomic potential and calphy.

Graph atomic cluster expansion for semilocal interactions beyond equivariant message passing

Atomic Cluster Expansion (ACE), which provides a formally complete set of local basis functions, has been extended to incorporate graph-based basis functions. This extension enables an efficient and physically transparent description of semilocal interactions. By simplifying the graph expansion through tensor decomposition, an iterative procedure emerges that aligns with modern message-passing machine learning interatomic potentials. This approach facilitates the incorporation of a large number of chemical elements and enables the parameterization of universal machine learning interatomic potentials (uMLIPs) using extensive datasets, such as the complete Materials Project or Alexandria. These foundational uMLIPs can simulate a wide range of materials with moderate accuracy out of the box while allowing efficient fine-tuning for improved accuracy in downstream applications.

A. Bochkarev, Y. Lysogorskiy, and R. Drautz,
Graph atomic cluster expansion for semilocal interactions beyond equivariant message passing,
Physical Review X, 14(2), 021036, 2024

AMS

4. 2. Atomistic Simulation of Mechanical Behaviour

Group leader:
Dr. Matous Mrovec

Group members:
Evgenii Fedorov
Minaam Qamar
Dr. Daria Smirnova
Dr. Sergei Starikov

▸ Research

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

The materials we are interested in include 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, perovskite oxides, and carbon based materials. The methods and models we employ span the whole atomistic modelling hierarchy from accurate first-principles methods through approximate electronic structure approaches to novel machine-learned interatomic potentials. Our main focus currently lies in 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.

▸ Competences

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

Simulations of pipe diffusion

Pipe diffusion (PD) along dislocations can play an important role for the self-diffusion at moderate temperatures in plastically deformed materials. We carried out a comprehensive investigation of PD mechanisms in several body-centered cubic (bcc) transition metals by means of large-scale atomistic simulations. We found that the PD mechanism in both screw and edge dislocations has an intrinsic nature associated with dynamical formation and migration of Frenkel pairs. However, different atomic structures of both dislocation cores are decisive for the character of the migration events, resulting in a very fast 1D diffusion along the screw dislocations and a slower 3D diffusion along the edge dislocations. The predicted PD coefficients are several orders of magnitude greater than the bulk diffusion coefficients, so that the dislocation diffusion needs to be considered when interpreting diffusion in plastically deformed metals at temperatures below half of the melting temperature. At high temperatures approaching the melting temperature, we observed a formation of additional defects such as jogs and kinks which require further investigation.

S. Starikov, V. Jamebozorgi, D. Smirnova, R. Drautz, and M. Mrovec,
Atomistic simulations of pipe diffusion in bcc transition metals,
Acta Materialia, 260, 119294, 2023

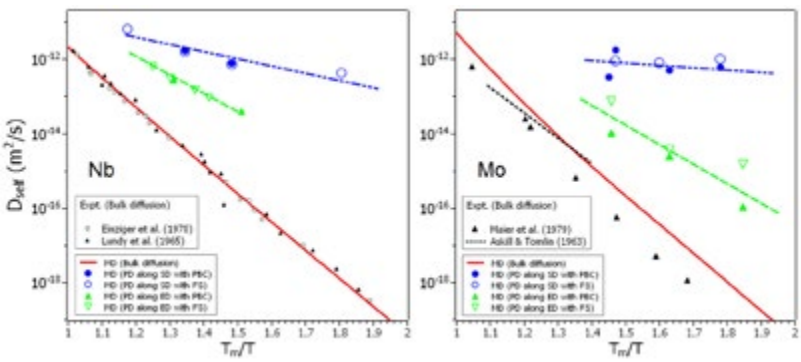

Fig. 4.4: The calculated PD self-diffusion coefficients for screw (SD) and edge (ED) dislocations in Nb (left) and Mo (right) plotted as a function of homologous temperature T/Tm in Arrhenius coordinates. Theoretical and experimental bulk diffusion coefficients are included for comparison.

Morphology of Pt-Rh nanoparticles for catalytic applications

Insight into structural and thermodynamic properties of nanoparticles is crucial for designing optimal catalysts with enhanced activity and stability. We developed an atomic cluster expansion (ACE) parametrization for the binary Pt-Rh system based on accurate electronic structure calculations. The ACE potential was applied in atomistic studies of Pt-Rh nanoparticles that are important for catalytic applications. We demonstrated that the Pt-Rh ACE is able to reproduce accurately a broad range of fundamental properties of the elemental metals as well as their compounds while retaining an outstanding computational efficiency. This enabled to carry out a direct comparison between predictions of atomistic simulations and observations made by high resolution transmission microscopy experiments. The simulation results show a strong preference for Pt segregation at surfaces of the nanoparticles, which is consistent with experimental observations. We also investigated nanoparticles with a core-shell morphology, as shown in *Fig. 4.5*. Based on MD simulations at elevated temperatures, we showed that the core-shell cluster morphologies consisting of a Rh core with a thicker Pt shell observed in experiments are not thermodynamically favorable but rather kinetically stabilized.

Y. Liang, M. Mrovec, Y. Lysogorskiy,
M. Vega-Paredes, C. Scheu, and R. Drautz,
Atomic cluster expansion for Pt-Rh catalysts: From ab initio to the simulation of nanoclusters in few steps,
Journal of Materials Research, 38, 5125, 2023.

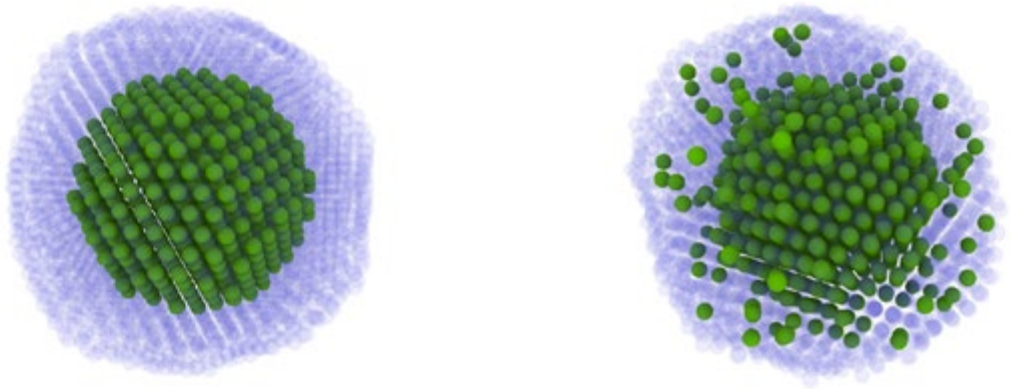

Fig. 4.5: Morphology of a core-shell nanocluster after 2 ns annealing at (a) 1000 K (left) and 1500 K (right). Rh atoms are in green, Pt atoms are in transparent blue. Taken from Ref. [2].

Non-collinear magnetic ACE for Fe

The atomic cluster expansion is not limited to representing energies as a function of atomic positions and chemical species, but can be generalized to vectorial or tensorial properties and to incorporate further degrees of freedom (DOF). This is crucial for magnetic materials with potential energy surfaces that depend on atomic positions and atomic magnetic moments simultaneously. We employed the ACE formalism to develop a non-collinear magnetic ACE parametrization for the prototypical magnetic element Fe. The model was trained on a broad range of collinear and non-collinear magnetic structures calculated using spin density functional theory. We demonstrated that the non-collinear magnetic ACE is able to reproduce not only ground state properties of various magnetic phases of Fe but also the magnetic and lattice excitations that are essential for a correct description of finite temperature behavior and properties of crystal defects.

M. Rinaldi, M., Mrovec, A. Bochkarev,
Y. Lysogorskiy, and R. Drautz,
Non-collinear magnetic atomic cluster expansion for iron,
npj Computational Materials, 10, 12, 2024.

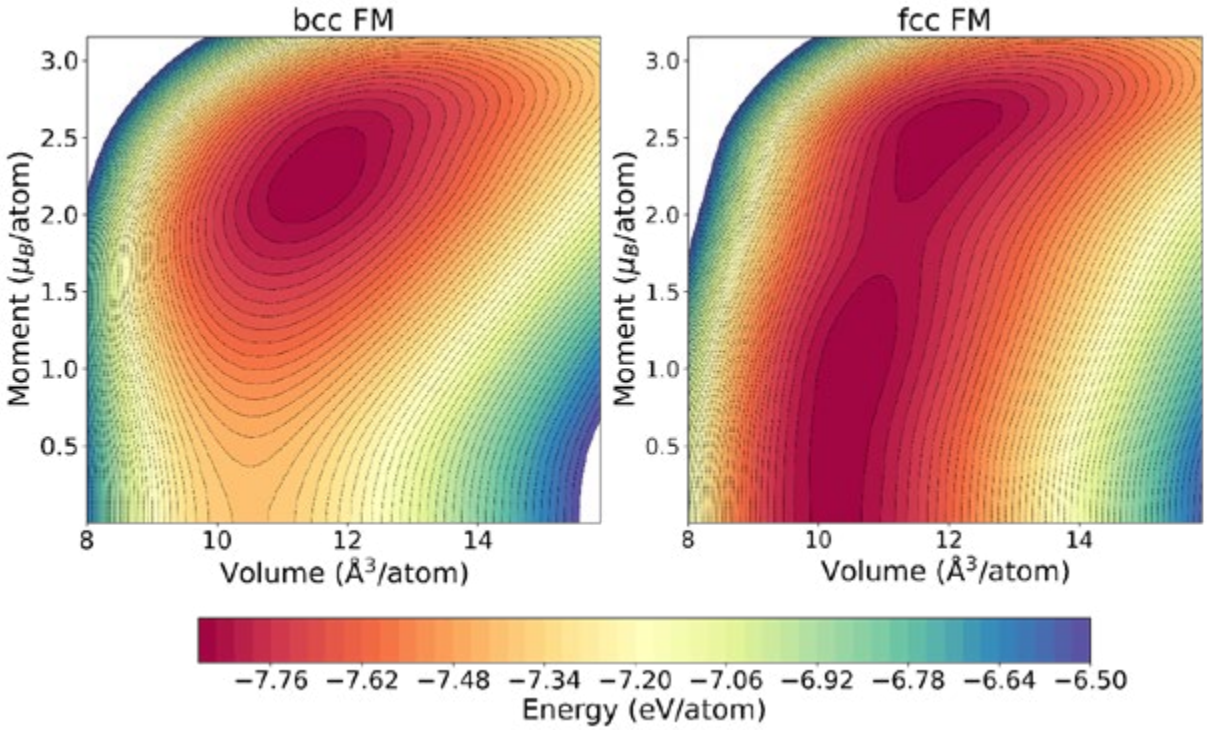

Fig. 4.6: Contour plots showing ACE predictions of the potential energy surface for the bcc (left) and fcc (right) ferromagnetic (FM) phases of Fe. Taken from Ref. [3].

AMS

4.3. Atomistic Simulation of Structural and Phase Stability

Group leader:
PD Dr. habil. Thomas Hammerschmidt

Group members:
Aleksei Egorov
Dr. Mariano Forti
Rohan Kumar
Isabel Pietka

▸ Research

The research group aims 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 and intermetallics), the complexity of the microstructures (e.g. hydrogen atoms at grain boundaries in steels) and the complexity of the physical phenomena (e.g. phase stability at finite temperatures).

Our portfolio of materials-science methods is based on electronic-structure calculations at the level of density functional theory (DFT) and coarse-grained descriptions of the electronic structure at the tight-binding level. These methods are combined with complementary data-driven methods using machine learning-based regression as well as machine learning interatomic potentials for exploring the influence of the local atomic structure and the local chemistry on structural and phase stability in multi-component alloys.

▸ Competences

- High-throughput density functional theory calculations
- Interatomic potentials based on physical models and machine learning
- Structure maps of d-d and p-d valent systems
- Descriptors of local atomic environments and machine learning
- Structural stability, point defects and interfaces in transition metals and their compounds compounds

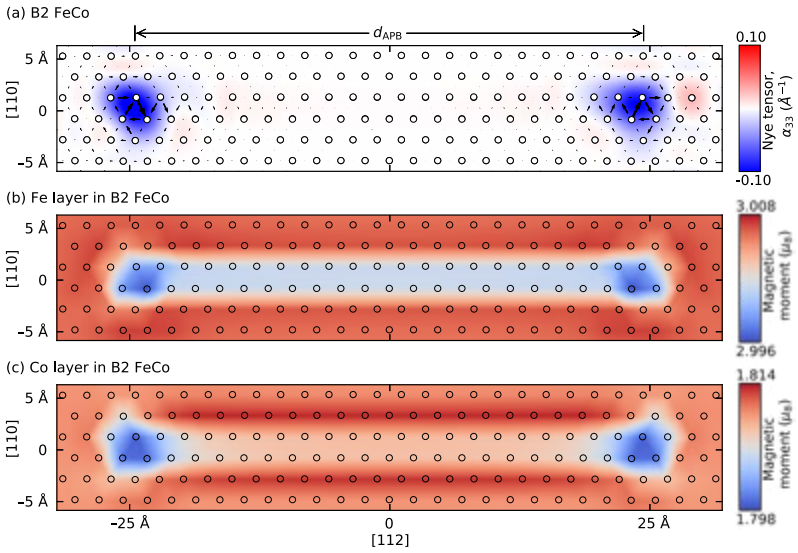

Fig. 4.7: The core structure of partial ½[111] screw dislocations in B2 FeCo we obtained with BOP. Partials separated by an antiphase boundary (APB) of the length dAPB=49Å. The differential displacement and Nye tensor distribution (a) reveal degenerate core structures. Additionally, the local magnetic moments of Fe and Co layers in B2 FeCo [(b) and (c)] display lower magnetic moments within the cores and APB, compared to bulk.

In this work, we elucidated the core structure of screw dislocations in ordered B2 FeCo using a recent magnetic bond-order potential (BOP) [Egorov et al., Phys. Rev. Mater. 7, 044403 (2023)]. We corroborated that dislocations in B2 FeCo exist in pairs separated by antiphase boundaries. The equilibrium separation is about 50 A, which demands large-scale atomistic simulations – inaccessible for density functional theory but attainable with BOP. We performed atomistic simulations of these separated dislocations with BOP and predicted that they reside in degenerate core structures. Additionally, dislocations induce changes in the local electronic structure and magnetic moments. This project was carried out in the International Max-Planck Research School SurMat with financial support from the Wilhelm and Günter Esser Foundation and the DFG-ANR Project MAGIKID.

A. Egorov, A. Kraych, M. Mrovec, R. Drautz,
T. Hammerschmidt,
Phys. Rev. Materials 8, 093604, 2024.

Exploration of complex intermetallic phases with machine learning

In this work we present a machine learning (ML) approach to perform a complete sampling of the chemical space of the complex R-phase in the Fe-Mo binary system with very high accuracy. This computation of the structural stability of this complex intermetallic is out of reach for DFT calculations due to the combinatorial explosion due to the large number of inequivalent lattice sites. To enforce reliable predictions, we train the ML models not only with conventional features of geometry and chemical composition but include also domain knowledge of details of the geometry and the interatomic bonds. With these ML models the structural stability of the Fe-Mo R-phase can be predicted for the first time across the full range of chemical compositions. This approach is currently rolled out for further multi-component compounds with experimental partners in the DFG-ANR project "Artificial Intelligence for Intermetallic Materials".

M. Forti, R. Drautz, T. Hammerschmidt,
(MRD newsletter 17, 2023, article in preparation).

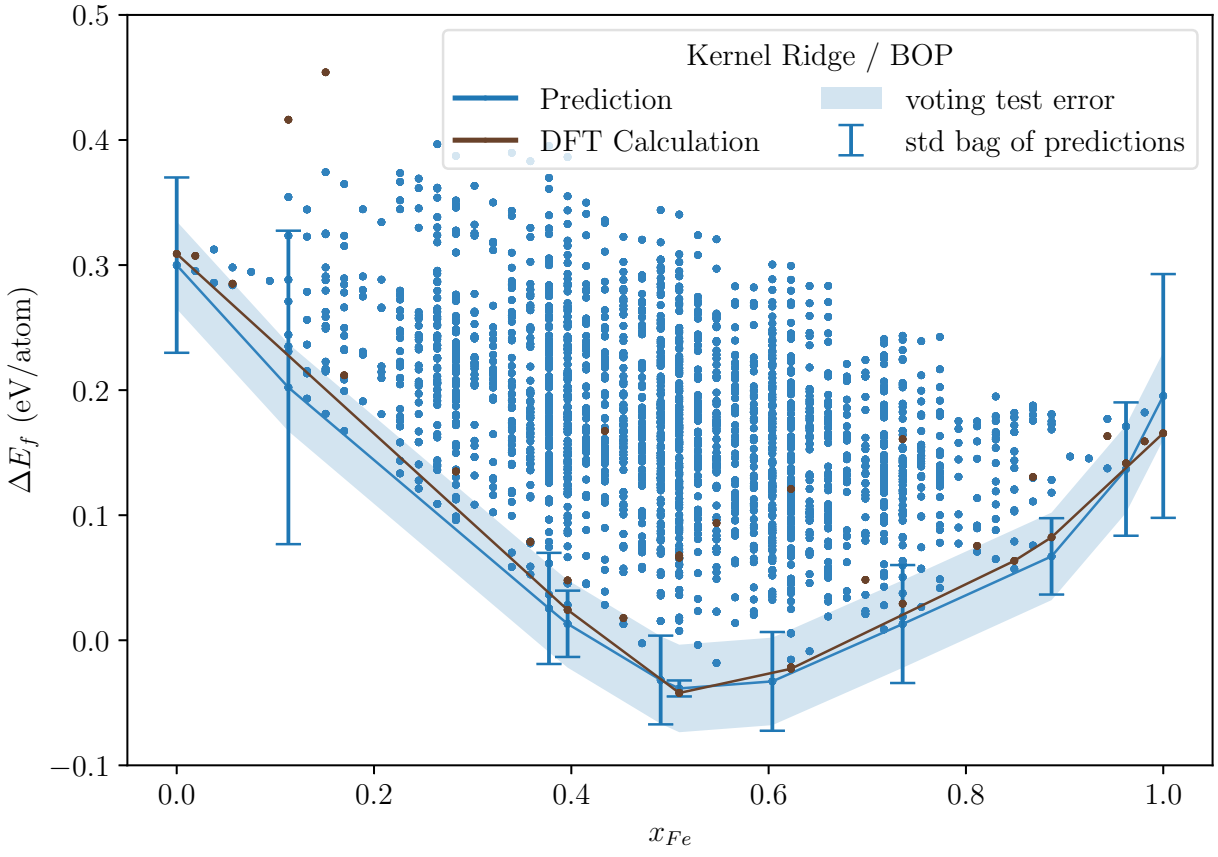

Fig. 4.8: Prediction of the formation energy of the R-phase in the Fe-Mo system across the range of chemical compositions including the expected precision around the convex hull.

ICAMS

Department Scalebridging Thermodynamic and Kinetic Simulation STKS

5. Department Scalebridging Thermodynamic and Kinetic Simulation

Prof. Dr. Ingo Steinbach

▸ Research

The department focuses 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.

Recently, the lecture "Phase-Field Theory and Application" given in the winter term has been published in a textbook "Lectures on Phase Field" by SpringerNature (https://link.springer.com/book/10.1007/978-3-031-21171-3); the compilation was co-authored by me and the research assistant Hesham Salama.

I. Steinbach, M. Uddagiri, H. Salama, M. Ali, O. Shchyglo, Highly complex materials processes as understood by phase-field simulations: Additive manufacturing, bainitic transformation in steel and high-temperature creep of superalloys,
MRS Bulletin, 49, 583–593, 2024

▸ Structure

The department's activities are organized in three 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)
- Diffusion in Metals and Minerals
  (Dr. Julia Kundin)

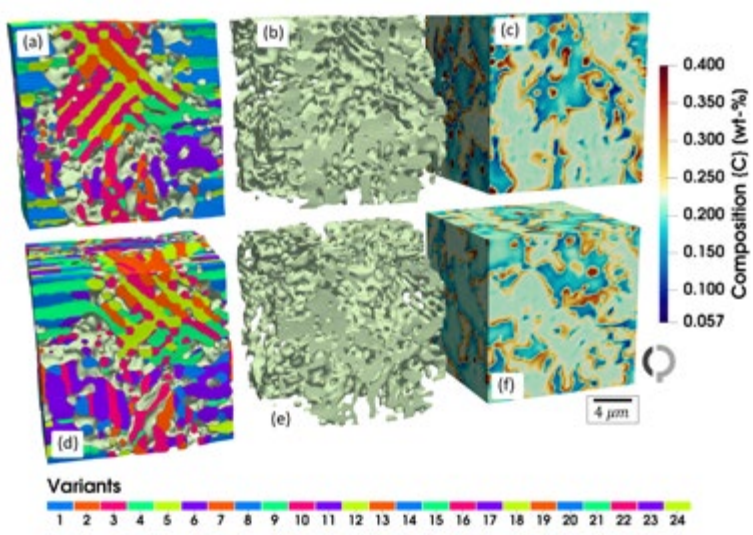

Fig. 5.1: (a, d) Bainitic microstructure, (b, e) retained austenite, and (c, f) carbon composition at heat extraction rates of 0.2 s−1 (a, b c) and 0.5 s−1 (d, e, f).

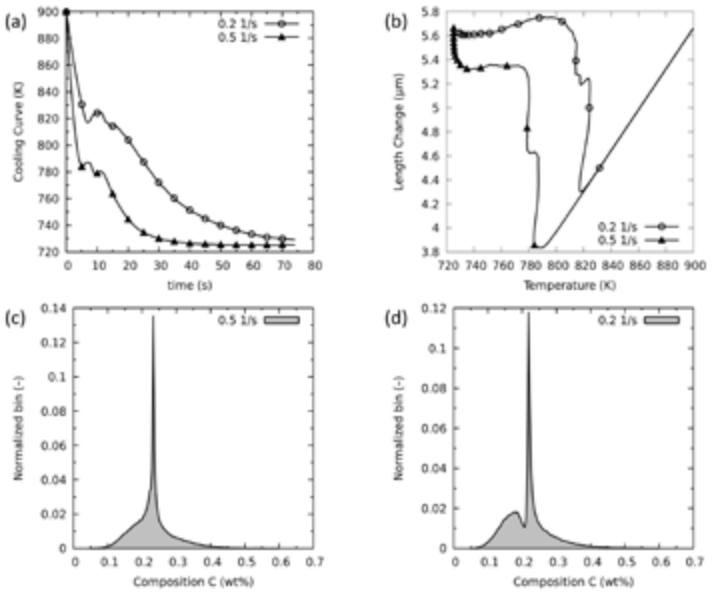

Fig. 5.2: (a) Cooling curves and (b) dilatometer curves calculated with heat extraction coefficients of 0.2 s−1 and 0.5 s−1. (c, d) Normalized bins of carbon composition calculated with heat extraction coefficients of 0.5 s−1 and 0.2 s−1, respectively. Bins are normalized by the total number of bins.

STKS

5.1. Phase-Field Simulations of Microstructures

Group leader:
Dr. Oleg Shchyglo

Group members:
Dr. Muhammad Adil Ali
Daysianne Kessy Mendes Isidorio
Dhanunjaya Kumar Nerella
Hesham Fathy Mohamed Ali Salama
Dr.-Ing. Marvin Tegeler
Dr. Murali Uddagiri

▸ Research

Our research group focuses on the development and application of new methods for phase-field simulations of microstructure development in complex materials. At present, the range of applications for phase-field modeling in our group includes rapid and conventional solidification, grain growth, eutectic and peritectic reactions, recrystallization, precipitation in industrial grade alloys, bainite and martensite formation in steel and many others. Nowadays, the phase-field method allows addressing not only the generalized microstructure formation scenarios in a qualitative manner but also real academic and industrial problems, showing good qualitative agreement with experimental observations. On top of that, the method provides access to the details of the microstructure formation, which are hard and sometimes not even possible to obtain experimentally. This makes the phase-field method indispensable when studying complex transformations involving the simultaneous evolution of a number of relevant fields, e.g. temperature, composition, stress and strain as well as the microstructure itself. The quintessence of the transformation complexity can be attributed to the formation of bainite in steel, where all fields mentioned above evolve simultaneously and have to be carefully considered. Together with the modeling of the martensite formation, the modeling of the bainite formation in steel is one of the focus areas of ongoing research in our group.

The group is actively developing the open-source phase-field simulation library OpenPhase, which is closely related to our scientific projects.

▸ Competences

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

Fig. 5.3: OpenPhase is an open-source software project targeted at the phase-field simulations of complex scientific problems involving microstructure formation in systems undergoing first order phase transformation.

Phase-field study of martensitic transformation in low-carbon steel

A comprehensive investigation of the complex interplay between martensitic transformation and plastic relaxation in low-carbon steels has been performed using advanced phase-field simulations. Our study, combining phase-field methodology with phenomenological crystal plasticity and utilizing a newly developed finite strain elasticity solver [1], revealed fundamental insights into the microstructure evolution during martensitic transformation [2]. The proposed approach enabled accurate consideration of large transformation-induced deformations and local lattice rotations. We systematically varied plastic slip rates from $1e^{-2}$ s^{-1} to $1e^{-6}$ s^{-1} and analyzed three carbon compositions (0.1, 0.2, and 0.3 wt. %) [3].

The simulations demonstrated several critical phenomena:

- There exists a critical threshold in the plastic relaxation rate that governs microstructure formation. Below this threshold, the steel's capacity for plastic deformation lags behind the martensitic transformation rate, resulting in a transition from fine uniform microstructures at higher plastic slip rates to elongated lath-like martensite structures at lower rates.
- The transformation-induced stress evolution exhibits an inverse relationship with the plastic slip rate. Quantitatively, slower plastic relaxation results in significantly higher internal stresses, ranging from 1.8 GPa at $\dot{\gamma} = 1e^{-2}$ s^{-1} to 5.2 GPa at $\dot{\gamma} = 1e^{-6}$ s^{-1}
- Carbon content emerges as a crucial factor in phase transformation behavior. Higher carbon levels stabilize the austenite phase and delay the martensite start temperature (Ms). Our simulated Ms temperatures of 497°C, 465°C, and 446°C for 0.1, 0.2, and 0.3 wt. % carbon, respectively, show excellent agreement with experimental observations.

This work advances our understanding of martensitic transformation kinetics in low-carbon steels by clarifying the competitive dynamics between rapid transformation at sonic speeds and slower plastic accommodation. These findings provide crucial insights for optimizing steel processing parameters and predicting resultant microstructures. The developed simulation framework offers a powerful tool for future investigations of phase transformations in complex metallic systems.

[1] O. Shchyglo, M. A. Ali, H. Salama,
Efficient finite strain elasticity solver for phase-field simulations,
npj Computational Materials, 10, 2024, p.52.

[2] H. Salama, O. Shchyglo, I. Steinbach,
The interplay between the martensitic transformation rate and the rate of plastic relaxation during martensitic transformation in low-carbon steel, a phase-field study,
npj Computational Materials, 2025

[3] H. Salama, M. A. Ali, O. Shchyglo, I. Steinbach,
Phase-field simulation framework for modeling martensite and bainite formation in steel,
Computational Materials Science, 241, 2024, p.113033.

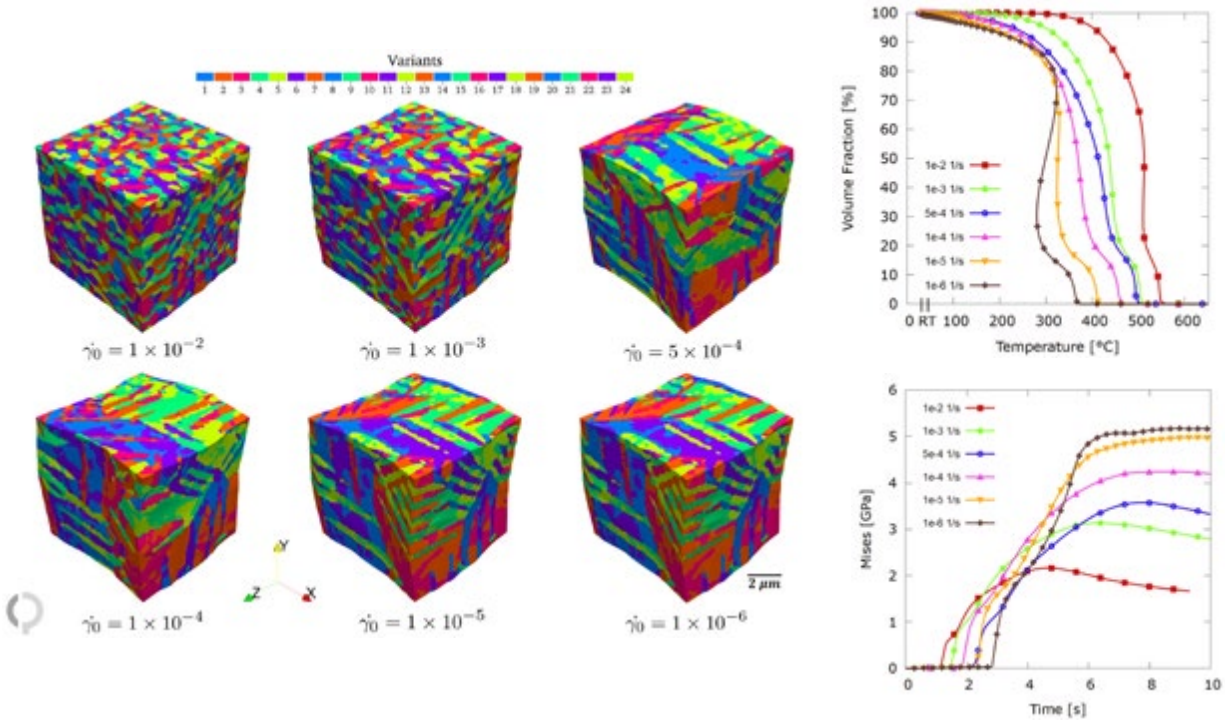

Fig. 5.4: Martensite microstructure, volume fraction and internal stress evolution considering different plastic slip rates.

Phase-field simulation of quaternary eutectic solidification

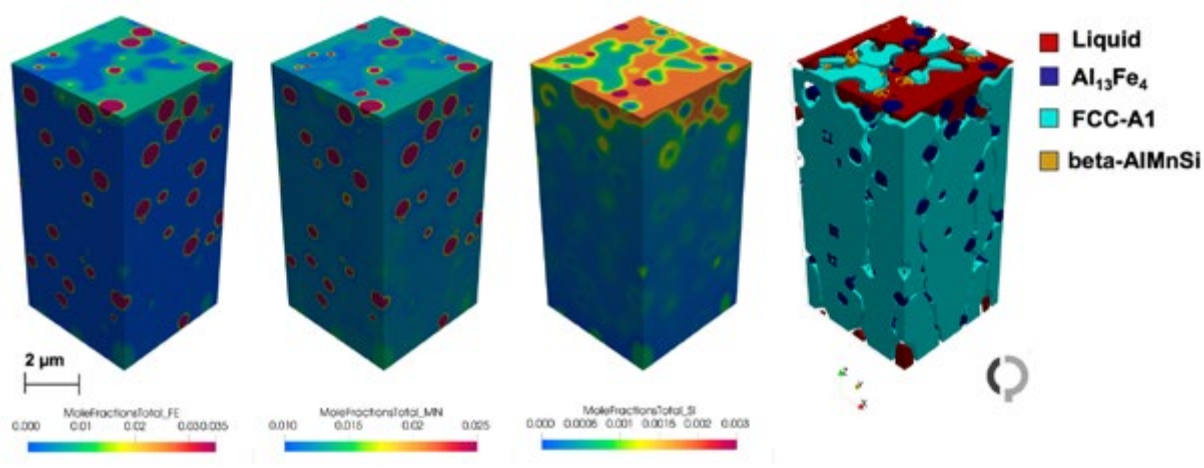

Fig. 5.5: Concentration distribution of all solute components in the multicomponent Al-Fe-Mn-Si system and the morphology with phase information.

With increasing environmental concerns and the rising demand for aluminium alloys, recycled aluminium is being explored as a sustainable option. However, controlling alloy composition and microsegregation is essential to prevent the formation of brittle intermetallic compounds that can weaken mechanical properties. To predict solidification behaviour and analyse the distribution of eutectic phases (FCC-A1, $Al_{13}Fe_4$, beta-AlMnSi) a microstructure evolution modelling in multicomponent aluminium alloy has been conducted using phase-field simulations coupled with CALPHAD thermodynamic databases. An Al-Mn-Fe-Si alloy with a nominal composition of Al-2.7%Mn-1.223%Fe-0.04%Si (wt%) has been investigated with a key focus on understanding the segregation of Fe, Mn, and Si in different phases. Simulations revealed a three-stage solidification process: $Al_{13}Fe_4$ nucleates first in the liquid, followed by the growth of lamellar or rod-shaped FCC-A1, and finally, beta-AlMnSi formed due to supersaturation of Mn and Si. Elemental analysis showed that Fe and Mn concentrate in $Al_{13}Fe_4$, while Mn enriches beta-AlMnSi and Si remains limited in FCC-A1 and beta-AlMnSi. It has been demonstrated that multicomponent diffusion plays a significant role, with Mn exhibiting high diffusion in beta-AlMn-Si, while Fe is depleted. By integrating phase-field simulations with CALPHAD data, this study provided valuable insights into phase evolution and elemental segregation, helping to optimize alloy compositions for improved mechanical performance, particularly in recycled aluminium applications [4].

[4] K. NouraniNiaki, M. Uddagiri, D. Isidorio, O. Shchyglo, and I. Steinbach,
Phase field simulation of Al-Fe-Mn-Si quaternary eutectic solidification,
Metals 15, no. 2, 2025,135.

Mechanical properties prediction of bainitic steel

Mechanical properties of bainitic steel have been evaluated via the computational modeling of steel microstructures, focusing on phase transformations, mechanical behavior, and yield surface estimation. The phase-field method was used to simulate optimal holding temperatures and cooling rates for controlled phase transformation. Different heat treatment processes were considered and studied to analyze morphological changes. Various isothermal holding temperatures were explored, and the results were compared with experimental data.

Microstructural features such as the thickness of the bainitic ferrite (BF) were calculated from both experiments and simulations under different heat-treatment conditions (450°C and 400°C). The average grain thickness at 450°C from simulations and experiments qualitatively aligned, whereas at 400°C discrepancies were observed between experimental and simulation results. Microstructures formed at 400°C exhibited finer grains with smaller sizes.

The tensile test simulations have been compared with experiments, and the Barlett91 yield surface has been constructed, providing additional insights into the mechanical behavior of steel under different conditions. The yield surface, which characterizes the material's elastic-plastic transition, has been constructed using stress-strain data and the corresponding material model. The Barlett91 yield surface provides a comprehensive representation of the anisotropic nature of the material, accounting for the directional dependence of yield stress in various loading conditions. This allowed for a more accurate prediction of the steel's behavior under real stress states.

This research integrated advanced computational techniques with experimental insights to optimize steel microstructures for industrial applications.

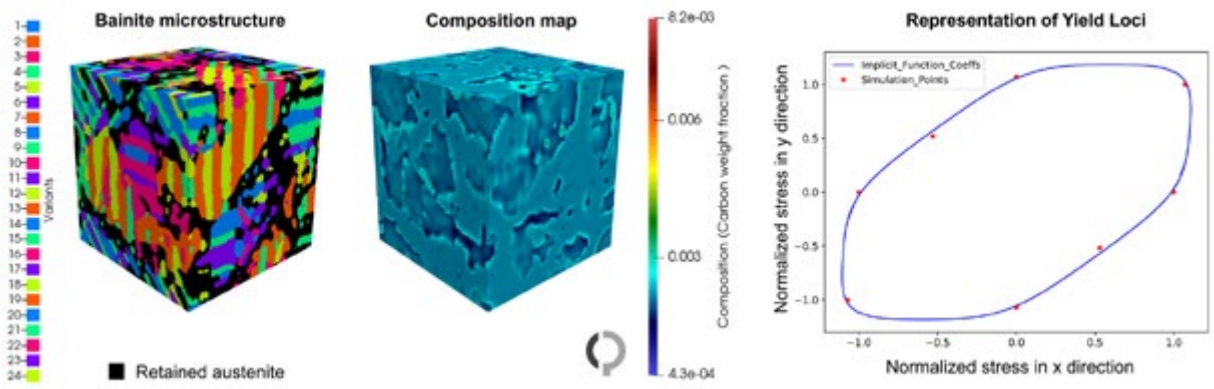

Fig. 5.6: Simulated bainite microstructure, carbon distribution and resulting yield surface.

5.2. Theory and Simulation of Complex Fluids

Group leader:
Prof. Dr. Fathollah Varnik

Group members:
Reza Namdar
Mohammad Norouzi
Hajar Tajedinisarvestani

▸ Research

The research interests of the complex fluids group encompass various physical phenomena in soft matter physics as well as gas dynamics in complex geometries. Recently, greater emphasis has been placed on the study of reactive gas flows through complex geometries within the framework of SFB287 (Bulk Reaction). To this end, a modified version of the lattice Boltzmann method has been employed, which accounts for large variations in fluid density. These density variations are not related to dynamic compressibility issues (since the Mach number is typically quite low in the applications relevant to this SFB) but rather result from heat generation due to chemical reactions. To extend the range of applications to solid combustion, a novel methodology has been developed by coupling the phase-field approach, which is renowned for its effectiveness in handling interfacial phenomena. This approach also broadens the applicability of the phase-field method to chemical reactions at interfaces.

Along this line, the volume averaging technique is used as part of the process to derive conservation equations for mass, momentum, and energy in the presence of a diffuse interface, thereby facilitating the coupling with the phase-field approach. As demonstrated in the examples below, the methodology has been thoroughly validated both numerically and experimentally. Furthermore, additional developments incorporating machine learning have been undertaken.

These studies involve collaborations with various research units, including expert colleagues both in Germany and abroad: Frank Beyrau (Head of the Institute for Fluid Dynamics and Thermodynamics, University of Magdeburg), Dominique Thévenin (Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg), the Automatic Control and System Theory group led by Martin Mönnigmann (Ruhr-University Bochum) and Benoid Fond (ONERA, Paris, France).

▸ Competences

- Modelling multiphase flows
- Mechanical response of amorphous materials
- Molecular dynamics of polymers
- Hybrid lattice Boltzmann-phase field modelling
- Numerical models to study combustion and heat transfer

Hybrid lattice Boltzmann-phase field modelling of heat transfer in gas flow through particle assemblies

The flow behavior and heat transfer of fluids/gases interacting with solid bodies is of great importance for industrial applications such as heat exchangers, cooling systems, biomass combustion, mixing and segregation, to name just a few examples. To address this interesting topic, we have recently proposed a hybrid computer simulation methodology to simulate heat transfer between a cold flow and an arrangement of hot cylinders [1]. An aspect of particular importance in the model regards thermal expansion of the hot gas, whose density varies beyond the domain of validity of the first-order Taylor expansion, the latter often referred to as the Boussinesq approximation. This is achieved by employing a modified lattice Boltzmann model which accounts for thermodynamic forces responsible for thermal expansion of the hot gas. Another feature of the method is the use of the phase field approach, which is well-known for its versatility and efficiency in dealing with physical processes at interfaces and the closely related kinetics of the phase boundary. As a benchmark test, this methodology is applied to study heat transfer in gas flow through a regular assembly of cylinders (*Figs. 5.6, 5.7*) and is successfully validated by comparison to experiments (*Fig.5.8*) [2].

Moreover, in a collaboration with expert colleagues on Deep Learning, we have provided training input-data to build up a data-driven reduced-order model (ROM) for predicting flow fields in a bed configuration of hot particles. The ROM consists of a parametric spatio-temporal convolutional autoencoder. The neural network architecture comprises two main components. The first part resolves the spatial and temporal dependencies present in the input sequence, while the second part of the architecture is responsible for predicting the solution at the subsequent timestep based on the information gathered from the preceding part (*Fig. 5.9*) [3].

[1] R. Namdar, M. Khodsiani, H. Safari, T. Neeraj, S. A. Hosseini, F. Beyrau, B. Fond, D. Thévenin, F. Varnik,
Numerical study of convective heat transfer in static arrangements of particles with arbitrary shapes: A monolithic hybrid lattice Boltzmann-finite difference-phase field solver,
Particuology 85, 186-197, 2024,
https://doi.org/10.1016/j.partic.2023.03.020.

[2] M. Khodsiani, R. Namdar, F. Varnik, F. Beyrau, B. Fond,
Spatially resolved investigation of flame particle interaction in a two dimensional model packed bed,
Particuology 85, 167-185, 2024,
https://doi.org/10.1016/j.partic.2023.03.011.

[3] A. Mjalled, R. Namdar, L. Reineking, M. Norouzi, F. Varnik, M. Mönnigmann,
Flow field prediction in bed configurations: A parametric spatio-temporal convolutional autoencoder approach,
Numerical Heat Transfer, Part B: Fundamentals, 1-24, 2024,
https://doi.org/10.1080/10407790.2024.2379006.

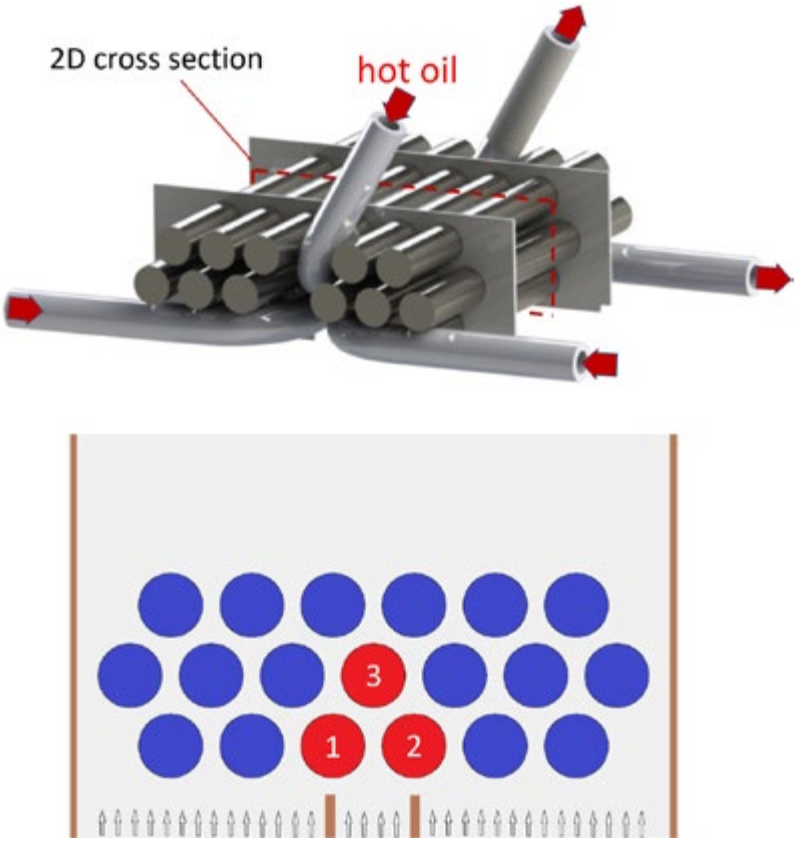

Fig. 5.6: Top: Schematic view of the experimental setup used in this study as a benchmark for numerical simulations. The three cylinders at the center are heated up by the flow of hot silicon oil. The surface temperature of these cylinders is 383 Kelvin. All other cylinders and the surrounding air are initially at room temperature. A gas enters the domain from the bottom at the ambient temperature (298 Kelvin). The dashed square highlights a two-dimensional cross section of the experimental setup, cutting the array of cylinders in the middle. Bottom: The simulation domain for the above experimental setup. The three red discs (labeled as 1, 2 and 3) represent the cross sections of the heated cylinders. The upward pointing white arrows indicate the inlet gas flow. The image is taken from Ref. [1].

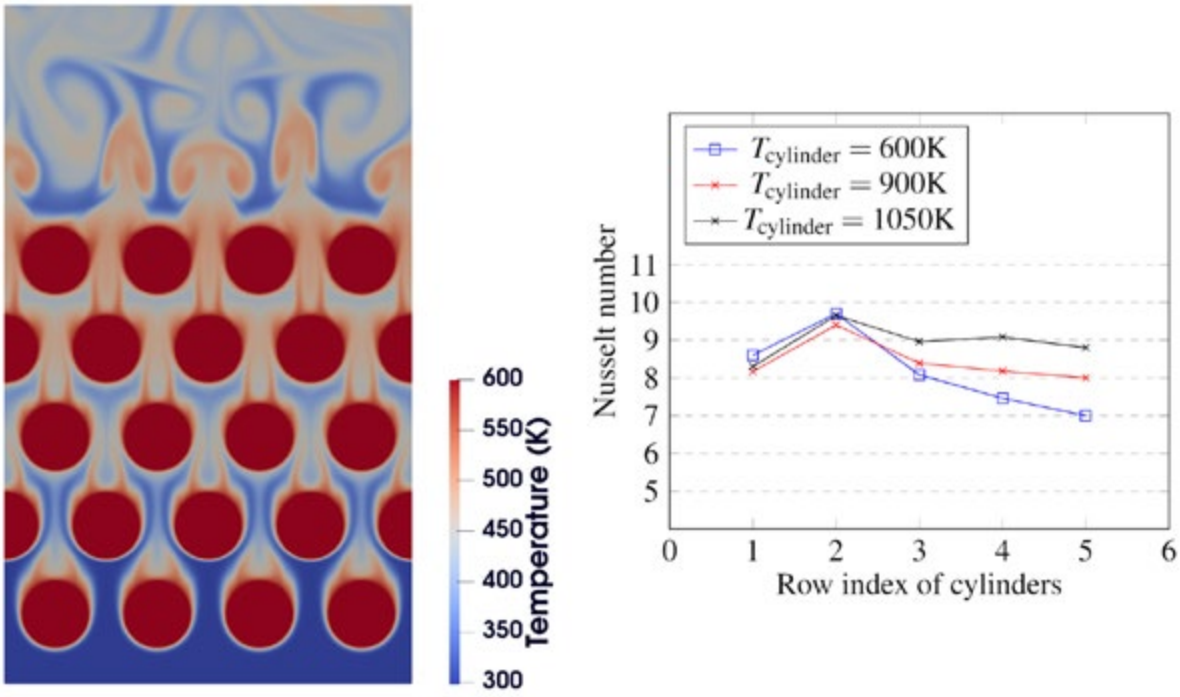

Fig. 5.7: Left: Temperature field during the flow of an initially cold gas through a regular assembly of hot cylinders. As the cold gas (blue color) moves upward, it receives heat from hot cylinders and becomes warmer (indicated by red color, see the color bar). All cylinders have the same constant temperature and thus act as identical heat sources. Right: The Nusselt number versus the row index for different cylinder temperatures as indicated in curve legends. The image is taken from the graphical abstract of Ref. [1].

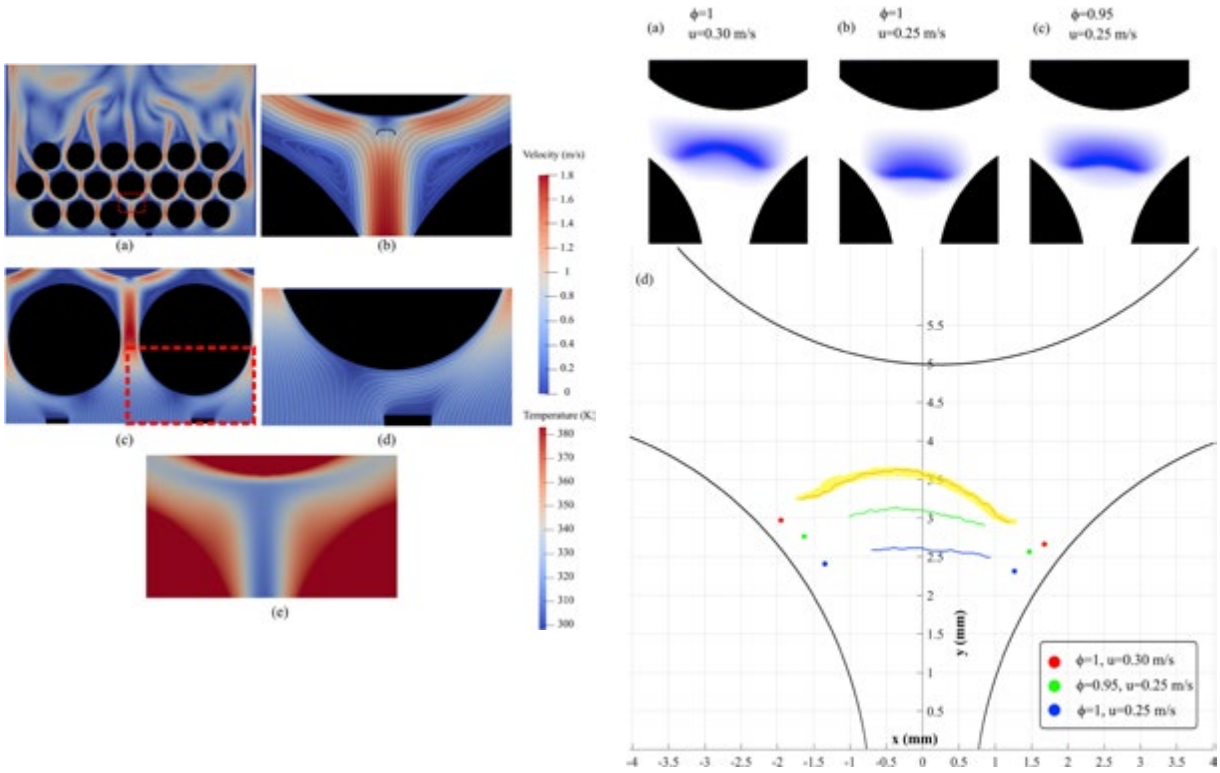

Fig. 5.8: Left: Simulation results in two dimensions for the velocity field in a gas flowing through a packed bed of cylinders. The domains marked by red rectangles in (a) and (c) are enlarged in (b) and (d), respectively. The temperature field is shown in (e). The cylinder temperature is set to 383 Kelvin. These data help identify the region, where a flame may be stable. Such a domain is highlighted by an arc in panel (b). Right: (a)-(c) Experimental flame chemiluminescence images recorded under different operating conditions as indicated in the legends; (d) The corresponding flame skeletons. Curved black lines on the top, left and right delineate the surface of the cylinders (note that the cylinder axis is perpendicular to the paper). The yellow region for the reference condition delineates the loci of all instantaneous flame front skeletons over the recording time. The dots mark the quenching point for each detected flame skeleton. The image is taken from Ref. [2].

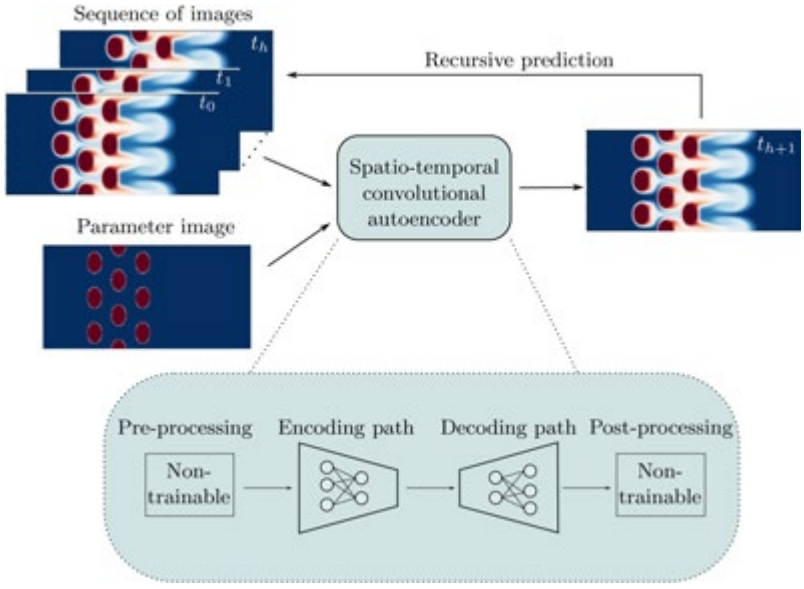

Fig. 5.9: A schematic representation of a data-driven framework for the parametric prediction of flow field simulations in a packed-bed configuration using a spatiotemporal convolutional autoencoder. Image courtesy of Ali Mjalled1 and Reza Namda2 [3].

STKS

5.3. Diffusion in Metals and Minerals

Group leader:
PD Dr. habil. Julia Kundin

Group members:
Dr. Ahmadreza Riyahi khorasgani
Micheal Younan

▸ Research

The activities of the DMM group mainly include modeling complex diffusion processes in metals and minerals on micro and meso scales described by continuum methods, e. g., by diffusion equations combined with phase-field theory. In this regard, our group deals with some critical phenomena such as grain growth, pore evolution, grain boundary diffusion and recrystallization, considering various factors such as inclusions, impurities, segregation on the grain boundary and elastic stresses. One of our research areas is grain growth in ceramics, which is accompanied by the pore evolution and grain boundary diffusion of dopants. Another aspect of our research concerns Kirkendall porosity occurring during interdiffusion in multi-component alloys resulting in a change of the mechanical properties. Once talking about minerals, simulation of texture evolution throughout solidification processes in the presence of the diffusion and convection effects in the liquid phase as well as nucleation events are of critical importance. All these processes in complex multi-phase systems can be modeled by combining different types of phase-field models and relevant diffusion models utilizing the modern thermodynamic and kinetic databases for the evaluation of diffusion parameters. The achieved numerical studies are supported by experimental data provided by the leading laboratories in Germany.

▸ Competences

- Phase-field modeling for diffusion chronometry in magmatic systems
- Grain-boundary diffusion in polycrystalline materials
- Automated assessments of atomic mobility parameters
- Diffusion couple modeling
- Phase-field modeling of Kirkendall pore growth in complex alloys

Carbon effect on thermo-kinetics of Co-Cr-Fe-Mn-Ni High entropy alloys

CoCrFeMnNi-based High entropy alloys (HEA), coined as Cantor alloys, as a new class of alloys are still under broad developments. In this work, interstitial alloying of carbon on the thermodynamics-kinetics coupling in this alloy is studied through CALPHAD and continuum approaches. First, phase diagrams and chemical potentials are calculated. Then carbon content- dependent mobilities of substitutional elements are modelled, based on experimental data. Consequently, a continuum model is applied to combine these properties in order to simulate interdiffusion HEA diffusion couples, underlining mutual influence of carbon and matrix elements diffusion on each other. The results are benchmarked against the experimental composition profiles. One important finding of this work is the discovery of the critical relevance of a correct accounting for the carbon-composition dependency of the atomic mobilities. Therefore, precise modeling of interdiffusion of substitutional elements requires considering interstitial elements-dependencies (here, carbon) of both thermodynamic factors and atomic mobilities. Additionally, noticeable up-hill diffusion of Chromium, depending on carbon content, is simulated accurately through tuning the strong thermodynamic interaction between carbon and chromium elements.

A. Riyahi khorasgani, J. Kundin, O. Lukianova, N. Esakkiraja, A. Paul, S. Divinski, I. Steinbach, Carbon effect on thermokinetics of Co-Cr-Fe-Mn-Ni high entropy alloys: A computational study validated by interdiffusion experiments, Acta Materialia. 261, 119358, 2023

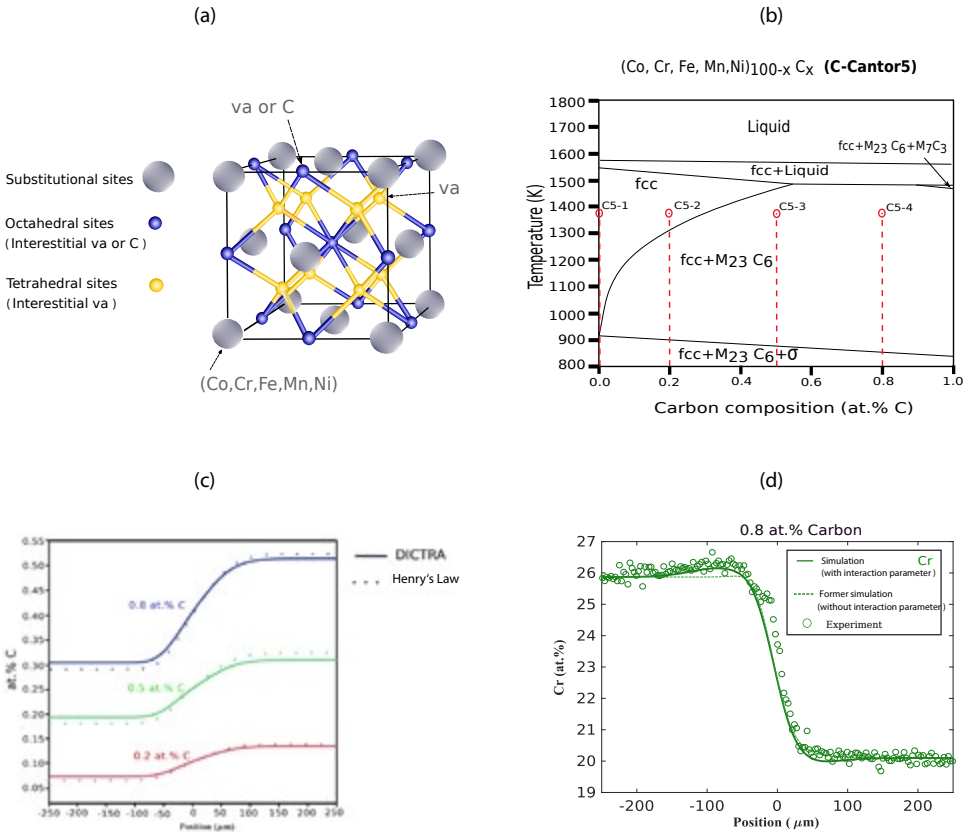

Fig. 5.10: Interdiffusion in CoCrFei/CoCrFeMnNiC diffusion couple. a) Two-sublattice model: the substitutional elements are shown as gray spheres (an "averaged" atom) and octahedral sites as positions for interstitial carbon and interstitial Va while tetrahedral sites occupy only interstitial Va. b) Temperature-composition sections of the calculated phase diagrams of C-Cantor5 systems based on the carbon content c) Carbon profiles simulated by DICTRA (solid lines) and using Henry's law approximation (dotted lines) for the couples with 0.2 at.%, 0.5 at.%, and 0.8 at.% of C add-ed to the right end member of the couples. d) Calculated Cr profiles (lines) in comparison with the experiment (symbols).

Phase-field modeling of kinetics of phase transformation in Ni-based superalloys under Gradient of composition

This work explores the kinetics of the phase transformation and the interdiffusion of elements and vacancies in single-crystal Ni-based superalloys, under isothermal annealing and composition gradient. The employed models in the present work exploit CALPHAD-based thermodynamics and kinetics databases, in order to perform realistic simulations. We specifically predict the interdiffusion of elements for a hypothetical alloy AlCoCrTaNi/Ni diffusion couple, equivalent to the CMSX-10/Ni diffusion couple, at 1323 K. Accordingly, the phase fraction and morphology of Gamma prime precipitations in the Gamma matrix is simulated as well. The implemented multi-component diffusion model takes into account vacancies and pore formation, reflecting Kirkendall effect. Furthermore, the time evolution of morphology parameters of the precipitate-depleted zone in the diffusive region are estimated.

A. Riyahi khorasgani, M. Younan, I. Steinbach, J. Kundin,
Phase-field modeling of kinetics of diffusive phase transformation in compositionally-graded Ni-based superalloys,
Journal of phase equilibria and diffusion,
Volume 45, pages 1055–1067, 2024

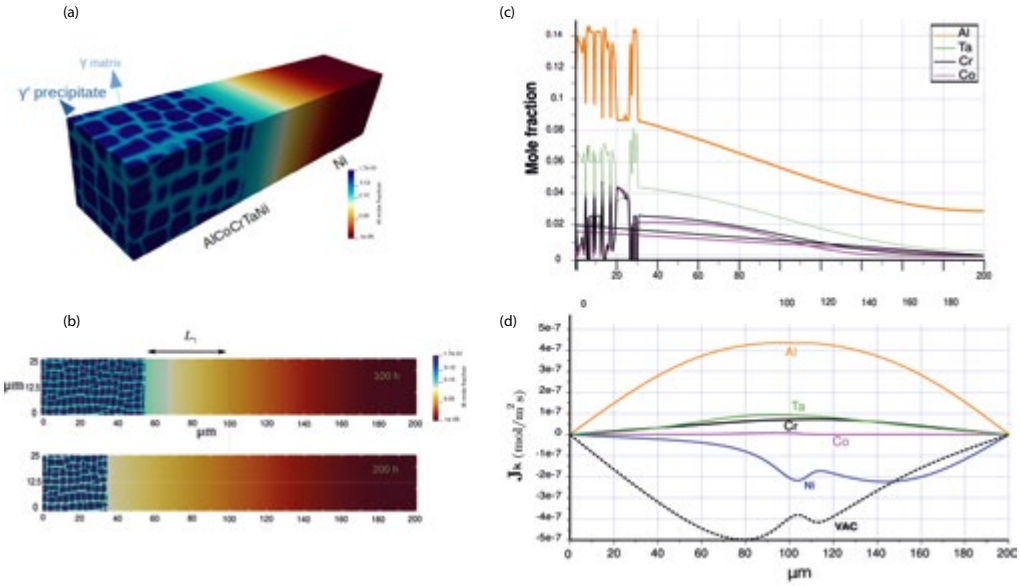

Fig . 5.11: 3D simulation of microstructure evolution in AlCoCrTaNi/Ni during annealing at 1323 K. Cuboidal coherent γ′ precipitates, rich in Al, are distinguishable inside γ-matrix. b) 2D simulations of dissolution of γ′ precipitates inside matrix. c) Simulation of interdiffusion profiles over middle scanning line for 200 h annealing at 1323 K. d) Simulation of fluxes of all elements and vacancies for 200 h annealing at 1323 K. the reduced site fraction of vacancies; the composition profiles of Mn; the predicted maximum pore fraction.

Modeling vacancy-induced porosity in compositionally-graded complex alloys

In the current work, a phase-field model of the void evolution is developed to investigate the vacancy-induced Kirkendall porosity within diffusion couples under isothermal annealing conditions. This model encapsulates a comprehensive computational framework for multicomponent diffusion, vacancy diffusion, voids growth, integrating considerations for surface anisotropy and morphological instability. This novel thermodynamically consistent methodology combines the phase-field model with the vacancy diffusion model and uses thermodynamic and atomic mobility parameters defined by CALPHAD approach. The generalized nature of the method enables us to include vacancies, covering all cases of non-ideal/ideal sinks and sources for vacancies, whether at dislocations or void surfaces. Moreover, the model can deal with compositionally complex alloys such as Ni-based superalloys. Along with the full model, a fast variant is also suggested, providing long-time simulations at the experimentally relevant time and space scales valuable for both academic and industrial contexts.

J. Kundin, Julia, A. Riyahi khorasgani, R. Schiedung, B. Camin, I. Steinbach,
Modeling vacancy-induced porosity in compositionally-graded complex alloys,
Acta Materialia 271, 119905, 2024

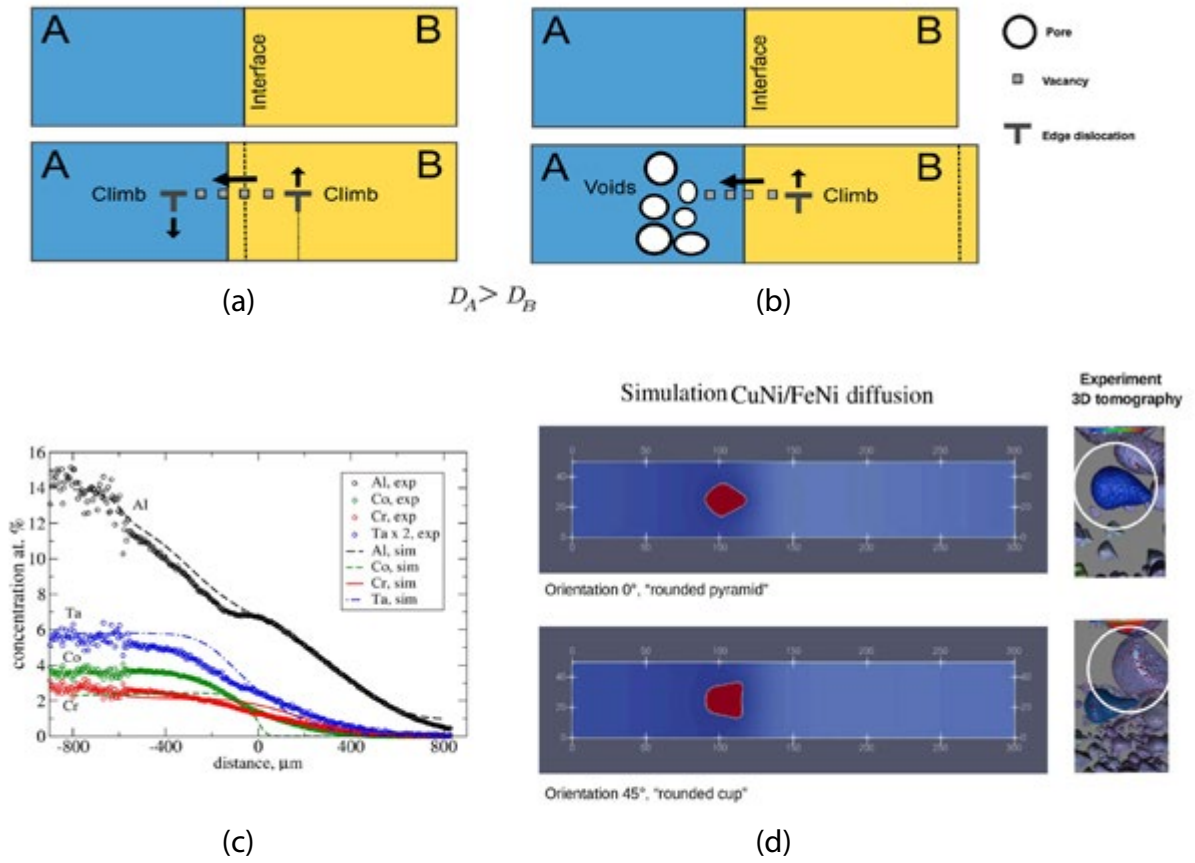

Fig. 5.12: Annihilation of vacancies at edge dislocations. b) Annihilation of vacancies at voids, c) Comparison of experimental interdiffusion profiles with calculated one by the standard diffusion model in 1D for the diffusion couple AlCoCrNi/Ni at 1523 K after 192 h. d) (left) Simulation results obtained by the fast MVE with 1 void in the CuNi/FeNi diffusion couple at 1523 K after 12 h. The crystal orientations are 0° and 45°. (right) 3D X-ray tomography in the CMSX10/Ni diffusion couple at 1523 K after 192 h. The white circles highlight the pores, whose shape is comparable to the simulation results. Matano plane is at z = 150 µm.

Morphological instability of Kirkendall voids in complex alloys

The present research explores theoretical and computational aspects of the morphological instability of Kirkendall voids induced by a directed flux of vacancies. A quantitative phase-field model is coupled with a multi-component diffusion model and CALPHAD-type thermodynamic and kinetic databases to obtain a meso-scale description of Kirkendall void morphologies under isothermal annealing. The material under investigation is a diffusion couple consisting of a multi-phase multi-component single crystal Ni-based superalloy on one side and pure Ni on the other side. The flux of the fastest diffuser in the superalloy, Al, towards the pure Ni causes a strong flux of vacancies in the opposite direction. This directed flux of vacancies leads to morphologically instable growth of voids. Phase-field simulations are performed in two (2D) and three dimensions (3D) to understand these instabilities, and the results are compared with experimental observations obtained by synchrotron X-ray tomography. Finally, the simulation results are analyzed with respect to the Mullins–Sekerka linear stability criterion.

A. Riyahi khorasgani, I. Steinbach, B. Camin, J. Kundin,
A phase-field study to explore the nature of the morphological instability of Kirkendall voids in complex alloys,
Scientific Reports Nature. 14, 30489, 2024

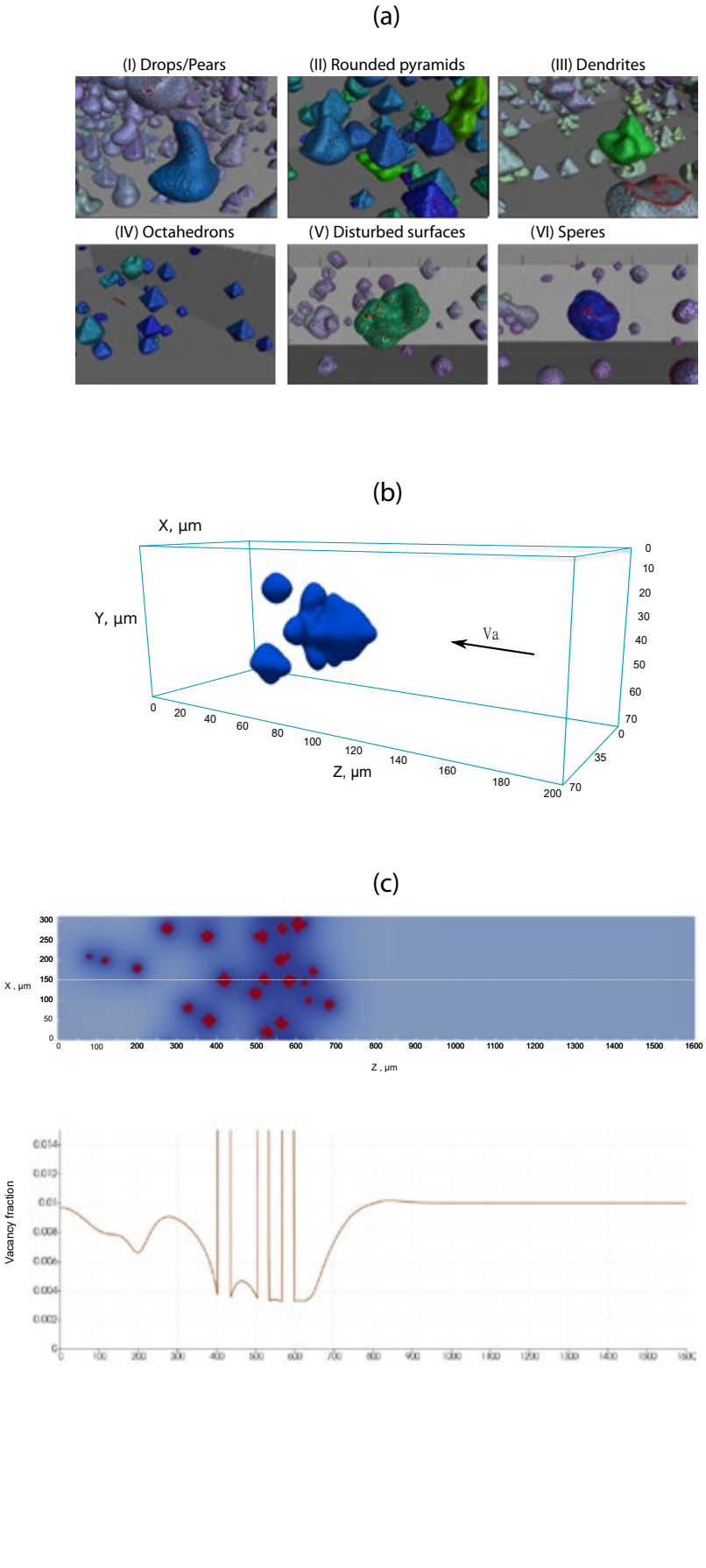

Fig. 5.13: a) X-ray tomography, exhibiting Kirkendall voids morphology at different sections in diffusion couple CMSX-10/Ni. b) 3D simulation of three neighboring Kirkendall voids after 255 hours annealing at 1523 K; Asymmetrical morphology of two pores behind the front dendrite pore is due to interaction among voids. c) 2D simulation of a real-size diffusion couple: 2D vacancy fraction field of vacancies and 1D vacancy fraction profile across the central scanning line.

ICAMS

Department Micromechanical and Macroscopic Modelling 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. The focus of research in the department Micromechanical and Macroscopic Modelling is to gain new insights into the relationships between microstructure and properties of technologically relevant materials using the methods of scale-bridging materials modelling. One goal of this work is to deepen our understanding of fundamental deformation and failure mechanisms and to predict macroscopic mechanical properties of materials. The strong dependency of these mechanisms and properties on the atomic structure and the microstructure of material results in the need for scale-bridging modelling. With respect to the macroscopic mechanical properties, we study strength under monotonic and cyclic loading, hardness, and fracture toughness in a wide range of environmental conditions such as varying temperatures and chemically aggressive media leading to corrosion and hydrogen embrittlement. The department's research activities can be divided into four areas with the following objectives:

1. **Micromechanical material models:** Investigation of microstructure-property relationships of technically relevant materials by statistically representative mapping of real microstructures in computer models and simulation of mechanical behavior under various mechanical-thermal-chemical loads with physically motivated material models; model validation by comparison of numerical results with experiment.

2. **Hybrid material characterization:** Combining experimental and numerical methods to determine and to describe material behavior on different length and time scales; exploring inverse methods to determine hidden parameters not directly obtainable from experiment by combining experiment and modelling.

3. **Data-oriented materials modelling:** Exploration of the necessary data structures to enable machine learning for surrogate models and digital material twins; efficient generation of large data sets by physically motivated micromechanical or atomistic models.

4. **Atomistic simulation:** Investigation of fundamental deformation and failure mechanisms at interfaces of metallic and intermetallic alloys using density functional theory and molecular dynamics; understanding the relationship between chemical composition, atomistic structure, and mechanical properties.

Fig. 6.1: Members of the MMM department at the end of 2024. From back to front and left to right: Vladimir Lenz, Rebecca Janisch, Nguyen Xuan Vu, Haris Ahmed Bhatti, Sidrah Sidrah, Eva Masuch, Hafiz Muhammad Sajjad, Yanling Schneider, Onur Can Sen, Alexander Hartmaier, Yousef Rezek, Ronak Shoghi, Feng Pan, Jan Schmidt.

The first research area is represented in the group "Micromechanical Material Models" that is currently headed by Prof. Alexander Hartmaier. The second research area has been supervised by Dr. Hafiz Muhammad Sajjad, who has left ICAMS in December 2024. We sincerely thank Dr. Sajjad for his contributions to research and teaching at ICAMS during the last years and briefly summarize the main results of his work below. The research topic "Data-Oriented Materials Modelling" is organized by Ronak Shoghi, who is currently a doctorate candidate at ICAMS. The activities on atomistic modelling within the department MMM are conducted in the group "Mechanical Properties of Interfaces" headed by PD Dr. habil. Rebecca Janisch.

One particular challenge in micromechanical materials modelling is the assessment of constitutive material parameters on the microscale. While macroscopic material properties can conveniently be gained by standardized materials testing methods, probing material behavior on the microscale poses many challenges. Basically, there are two micro- or nanomechanical testing methods that are established within the community: instrumented indentation and pillar compression. Throughout the years, we have gained a lot of expertise at ICAMS on extracting proper material parameters from indentation methods from the nanoscale, over microscale indentation to macroscopic standard hardness tests. Such indentation tests can be conducted with a comparatively small effort compared to pillar compression tests and represent a quasi-non-destructive method that can also be applied to finished components. However, the amount of information gained by indentation experiments is limited to a hardness value and – based on theoretical models – an elastic coefficient of the investigated material. The combination of experiment and numerical simulation in the form of a hybrid method offers the possibility to extract complete sets of material parameters from indentation tests. This is accomplished by performing an inverse analysis, where a finite element model (FEM) of the indentation test is created based on guessed material parameters. The FEM results are then quantitatively compared with the experimental data, and the material parameters of the model are varied in an iterative procedure until the optimal agreement between simulation and experiment is established. At this point, the model parameters represent the true material behavior. In the work of Dr. Hafiz M. Sajjad, in collaboration with an industrial partner, the possibilities of this inverse analysis of indentation data have been vastly extended to cyclic indentation, which allows us to extract material parameters that describe cyclic plasticity of materials and their fatigue behavior, see *Fig. 6.2*.

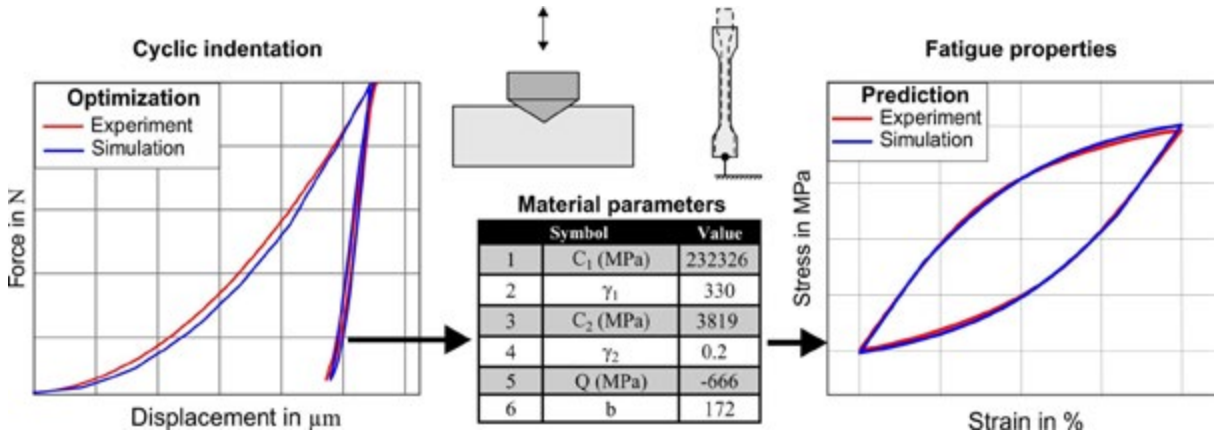

Fig. 6.2: The force-displacement curve of a cyclic indentation experiment (left) is used as input data for the inverse analysis, which results in material parameters for cyclic plasticity (middle). With these parameters, the material behavior under fatigue testing can be predicted. (Sajjad, Chudoba, Hartmaier. Materials 17 (2024) 3938.)

MMM

6.1. Mechanical Properties of Interfaces

Group leader:
PD Dr. habil. Rebecca Janisch

Group members:
Haris Ahmed Bhatti
Onur Can Sen
Farnoosh Ghaderi
Akshaya Karusala
Muhamad Yousuf Parhiyar
Timo Schmalofski

▸ Research

Segregation and crack propagation at interfaces significantly impact the strength and deformability of polycrystalline microstructures in metals and alloys. The "Mechanical Properties of Interfaces" research group studies such processes on a fundamental level, using atomistic simulations and ab-initio electronic structure calculations. We predict the energy, strength, and effective modulus of interfaces and defects in pure metals and metallic alloys. From these properties and their changes upon solution and segregation of alloying elements as well as tramp species, we derive trends and mechanisms, which help to understand and optimize the mechanical behaviour of microstructures. In addition to these quasi-static calculations, large-scale molecular dynamics simulations reveal the fundamental mechanisms of deformation and crack propagation in interface-dominated microstructures. By combining atomistic methods with statistical assessments, we survey structures throughout the parameter space, to derive further structure-property relationships.

In 2023/2024 the research projects of the group included hydrogen solubility and embrittlement in ferritic steel, including the description of alloying effects and the chemo-mechanical coupling of H segregation and deformation at grain boundaries. A second branch was the deformation and fracture of TiAl alloys. Furthermore, method-development oriented projects focussed on a multidimensional sampling of the grain boundary parameter space and grain boundary structure analysis.

▸ Competences

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

Interface effects on deformation and fracture in fully lamellar Ti-Al alloys

Strengthening of metals by incorporating nano-scale twin boundaries is a promising approach to overcome the strength-ductility trade-off of metals and metallic alloys. Nano-lamellar microstructures of lightweight Ti-Al alloys show a great potential and are already being used in high temperature applications. However, for designing optimal microstructures, the contribution of the interfaces to the overall deformation and fracture behavior needs to be better understood.

The interfaces in lamellar Ti-Al can act as barrier for lattice dislocations, but also as dislocation source. Unless they are perfectly coherent, they exhibit misfit and/or compatibility stresses and are likely to nucleate cracks and alter crack paths. We have investigated deformation and fracture by means of large-scale atomistic simulations to clarify whether the different boundaries in lamellar Ti-Al are effective and equal strengtheners and in particular, what is the role of the interface coherency in these processes.

We observed that all internal boundaries increase the fracture toughness – in particular the semi-coherent ones - although the crack-tip mechanisms differ and there is a strong directional anisotropy. This can be seen in *Fig. 6.3*, where the advancement of a penny-shaped crack in the vicinity of different interfaces is shown. In almost all cases it is less than in the perfect single crystal (labelled as γ). The minimum advancement is observed for the semi-coherent (SC) or partially semi-coherent (PSC) interfaces. At a semi-coherent, so-called "Pseudotwin" (PT) interface the misfit interfacial dislocations cause nucleation events, as shown in *Fig. 6.4* . These events are responsible for lowering the overall dislocation nucleation stress and cause localized or early plasticity. While this could be detrimental to the tensile strength of a lamellar sample, it does improve its fracture toughness by dissipating energy without further crack advancement.

Summarizing, the degree of lattice misfit of/at lamellar interfaces in two-phase Ti-Al alloys governs dislocation nucleation at the interfaces and therefore represents an important material parameter, which can also be adjusted experimentally, e.g. by varying the processing route as well as the chemical composition.

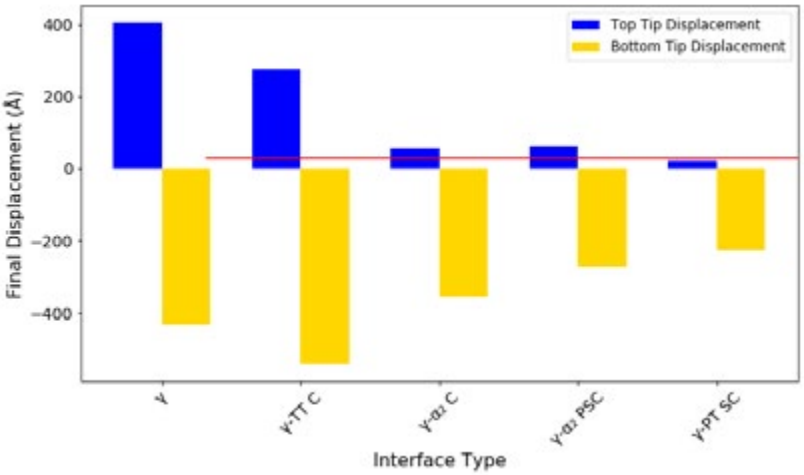

Fig. 6.3: Crack advancement of a penny-shaped crack under tensile load. The crack was initiated in the vicinity of an interface, the position of which is marked by the red line. The crack advancement in an ideal γ-TiAl single crystal is shown for comparison. The interfaces are the intrinsically coherent γ/γ true twin (γ-TT C), the strained and coherent γ-TiAl/α_2-Ti_3Al interface (γ-α C), the partially relaxed and semi-coherent γ-α_2 interface (γ-α_2PSC), and the semi-coherent γ-TiAl pseudo-twin (γ-PT SC). The diagram shows that the semi-coherent interfaces are effective in blocking the crack propagation.

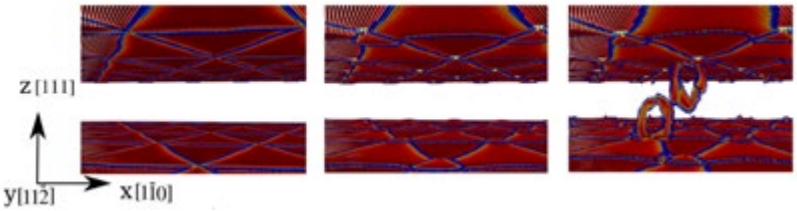

Fig. 6.4: Three snapshots of an atomistic simulation of a TiAl lamella under strain. Since perfectly coordinated atoms have been deleted, most of the lamella interior is shown as empty space. The lamella is bordered by two PT interfaces. Atoms are colored according to centrosymmetry. Blue atoms mark the dislocation lines of the misfit dislocation network and red atoms the stacking fault region in between. The sequence shows how the network deforms under strain and finally nucleates dislocation loops into the lamella.

Hydrogen solubility and hydrogen-enhanced decohesion of ferritic steel grain boundaries

Hydrogen-enhanced decohesion (HEDE) is one of the many mechanisms of hydrogen embrittlement, a phenomenon that severely impacts structural materials such as iron and iron alloys. Grain boundaries (GBs) play a critical role in this mechanism, where they can provide trapping sites or act as hydrogen diffusion pathways.

The interaction of H with GBs depends on several factors, such as the H concentration, the H chemical potential, the local structure and chemical environment at the GB, and last not least the stress state of the interface, either during deformation or due to residual stresses in the microstructure. Ideally, a generalized solution energy in conjunction with the cohesive strength as function of hydrogen coverage shall be provided, which takes all these parameters into account. In our research group, we carry out density functional theory calculations to determine such relationships.

To identify segregation sites at special GBs in bcc Fe without the need to run the actual DFT calculation for every possible H position, a method based on a Voronoi analysis was proposed and validated via calculations of the solution energy (*see Figure 6.5*). Using this method, a series of calculations for different GBs, strain states and alloy and different compositions were carried out. At higher local concentrations, H leads to a significant reduction of the cohesive strength of the GB planes in all cases, but more pronounced in open than in close-packed GB structures. Mn as an alloying element was identified as a likely candidate to at least partially compensate this effect. Interestingly, the relative solution energy at different interfaces changes during mechanical loading. This suggests that, under certain conditions, stresses in the microstructure can lead to a redistribution of H from one grain boundary to another, which could provide an interesting route for microstructural design.

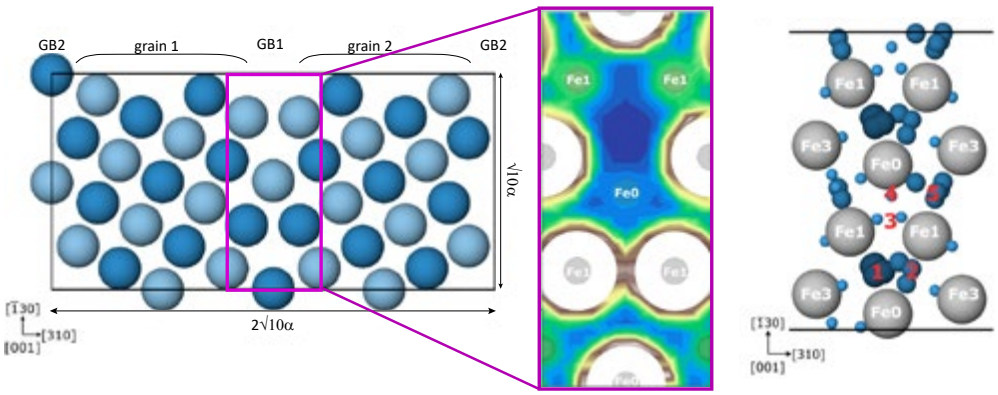

Fig. 6.5: Atomistic model of a special tilt grain boundary. The middle panel shows the solution energy of H in such a GB in bcc iron as obtained from DFT calculations. Blue are regions of low energy. These regions correspond to the clusters of voids which are obtained by a Voronoi analysis of the structure.

MMM

6.2. Micromechanical Material Models

Prof. Dr. Alexander Hartmaier

▸ Research

A combination of inverse analysis of nanoindentation data and micromechanical modelling, where the microstructure of a material is modeled in the form of a representative volume element (RVE), has been used very successfully in a collaboration with the groups of Professor Ghazal Moeini (Westfälische Hochschule Gelsenkirchen) and Professor Thomas Niendorf (Universität Kassel). In this work, a material obtained from additive manufacturing has been welded to a cast aluminum alloy by friction stir welding. The material response to cyclic loads has been determined by cyclic indentation tests and additionally by fatigue tests on small samples on the millimeter scale. Furthermore, the microstructure of the different regions of the joint component, i.e. as-cast material, additively manufactured material, and weld region, has been characterized by electron backscatter diffraction (EBSD) in the scanning electron microscope. Based on the local microstructure data, RVEs for the different regions of the hybrid welded material have been constructed, reflecting the specific microstructure characteristics in each region individually. Due to the high lateral resolution of the nanoindentation method, also the material parameters could be extracted locally for each individual region. In consequence, a fully parameterized microstructure model for the different regions in the welded material could be developed and validated against the results of miniature fatigue tests, see *Fig. 6.6*.

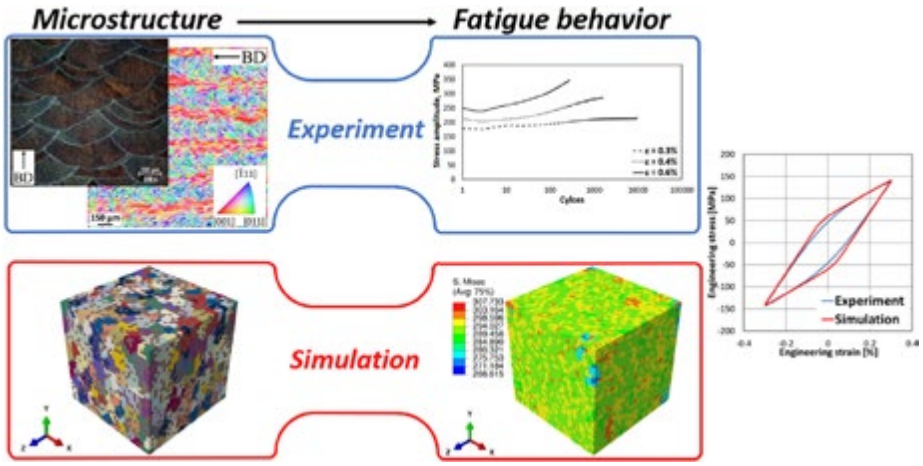

Fig. 6.6: Schematic view of the combination of experimental data of microstructure and mechanical properties of additively manufactured material (BD – build direction) (top) and microstructure-based modelling (bottom) to predict the macroscopic cyclic response of a material (right). (Rajan, Krochmal, Shahmardani, Wegener, Hartmaier, Niendorf, Moeini. Materials Science & Engineering A 879 (2023) 145232.)

MMM

6.3. Data-Oriented Material Modelling

Ronak Shoghi

▸ Research

In the last years, 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, have become an indispensable part of our research. In order to share data among different scientists of various backgrounds, it is mandatory to store data in a FAIR (Findable, Accessible, Interoperable, Reusable) way, which requires a semantic description of the data sets to be stored alongside the raw data itself. Such complex data structures can only be implemented into the daily practice of research labs if the data collection is achieved in a highly automized way with only minimal input requirements for individual users. In recent work, a dataschema that fulfills the FAIR requirements and at the same time includes a highly automized data collection along numerical workflows has been proposed to the community, see *Fig. 6.7*. This data schema is mainly applied to simulations of the mechanical behavior of polycrystals but can also be generalized to other purposes.

The long-term objective of these research activities is the development of a toolbox that allows users to generate digital material twins from rather simple experimental tests that are then augmented by data from fundamental numerical models. This data is used to train machine learning models of the material behavior under any thermal and mechanical boundary conditions that take over the role of conventional constitutive rules.

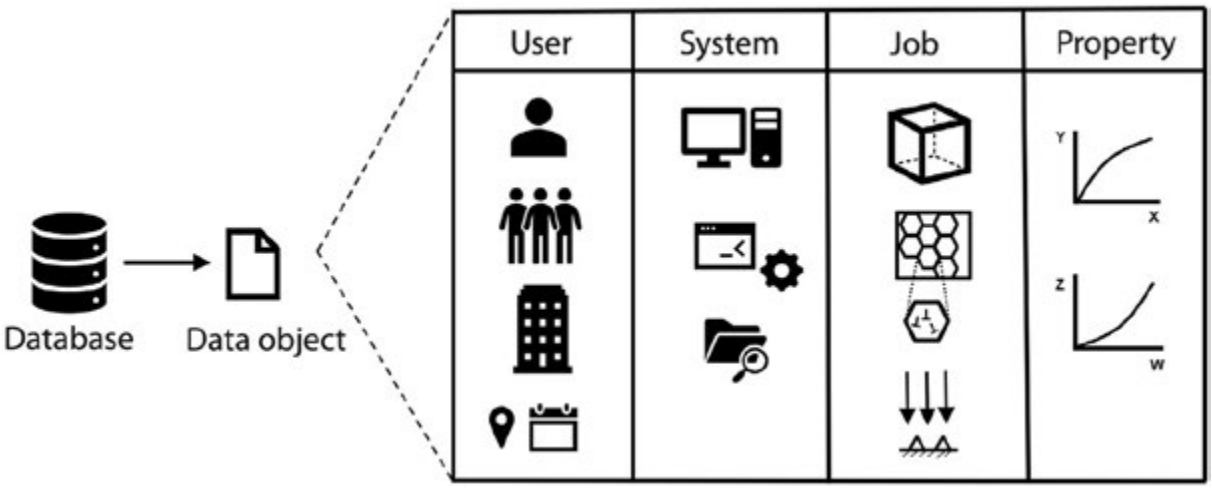

Fig. 6.7: Schematic view of the structure of a FAIR data object, that combines information about the users or owners of the data, the system on which this data has been generated, the software tools and their parameters that have been used to generate the data and the data about the material behavior itself. (Shoghi, Hartmaier. Adv. Eng. Mater. 27 (2025) 2401876)

ICAMS

Department Artificial Intelligence for Integrated Material Science AIIMS

7. Department Artificial Intelligence for Integrated Material Science

Group leader:
Prof. Dr. Miguel Marques

Group members:
Thalis Bispo Da Silva
Dr.-Ing. Théo Cavignac
Dr.-Ing. Pierre-Paul De Breuck
Antoine Loew
Sumit Mondal
Haichen Wang

The year 2024 marked significant advances in our understanding and prediction of conventional superconductors through the combined application of machine learning techniques and high-throughput first-principles calculations. Our group at ICAMS made substantial contributions to this field through several interconnected studies that significantly expanded both the available datasets and our predictive capabilities.

We developed ALEXANDRIA, an open database containing more than 5 million density-functional theory calculations for periodic three-, two-, and one-dimensional compounds. This extensive dataset provides a firm foundation for training machine learning models in materials science. Our systematic approach involved using crystal graph attention networks to predict compounds near the convex hull and universal machine learning interatomic potentials for preliminary geometry optimizations. This strategy proved increasingly effective with each iteration, as demonstrated by the growing proportion of compounds found below 0.1 eV/atom from 42.6% in the first round to 74.8% in the third round.

Building on this foundation, we conducted a large-scale study of conventional superconducting materials using a machine-learning accelerated high-throughput workflow. Starting with the creation of a comprehensive dataset of around 7000 electron-phonon calculations, we developed robust machine learning models capable of predicting electron-phonon and superconducting properties based on structural, compositional, and electronic ground-state properties. This approach led to the identification of 541 compounds with transition temperatures surpassing 10 K, encompassing a variety of crystal structures and chemical compositions.

Perhaps our most significant discovery was the layered metal $LiMoN_2$, which we predicted to have a transition temperature of approximately 38 K. This material exhibits extreme electron-phonon coupling between the electrons participating in the very strong covalent bonds within the MoN_2 layers, with almost all N and Mo phonon modes contributing equally to a remarkably high coupling constant of $\lambda = 1.9$. The material exhibits three different superconducting gaps but, contrary to MgB_2, superconductivity seems to arise mainly from interband coupling.

We also made significant progress in improving the accuracy of machine-learning models through the strategic use of force constants. Our implementation of training on force constants in the NequIP model, utilizing the auto-gradient of total energy with respect to atomic positions, has shown promising results in predicting phonon properties while reducing the number of structures needed for neural network training. This advancement was demonstrated through detailed studies of the Ti-Nb-Ta and Li-B-C ternary phase diagrams (*see Fig. 1*).

Looking ahead, our work opens several promising avenues for future research. The synergy between machine-learning techniques and conventional density-functional based approaches holds great potential for a systematic exploration of the multinary phase diagram, enabling the search for superconducting compounds at high temperatures, and even room temperature. Furthermore, the availability of more data will inevitably make machine learning models more precise, in a virtuous cycle that will allow the community to investigate conventional superconducting properties of all possible stable materials, both at ambient pressure and under pressure.

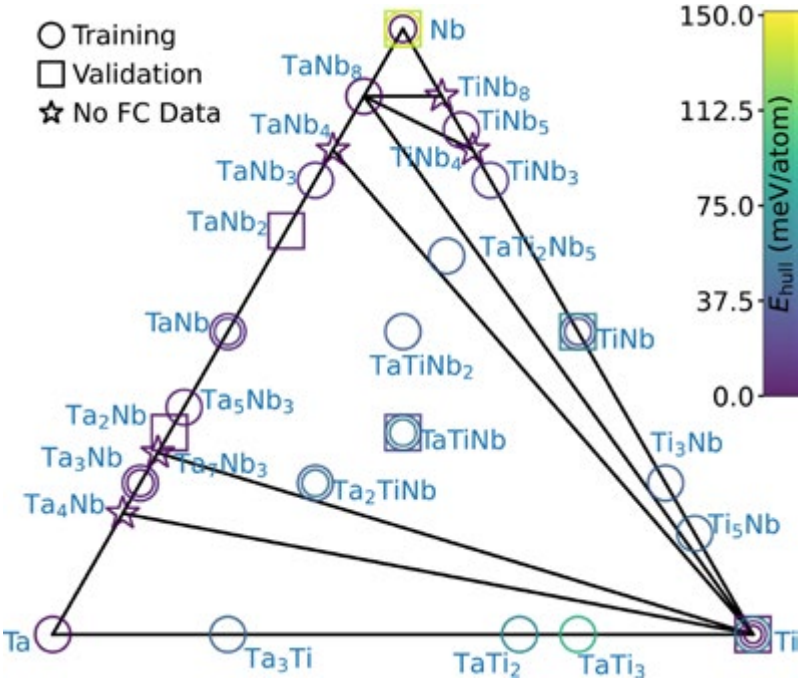

Fig. 7.1: Phase diagrams of Ti-Nb-Ta systems showing the compounds used for training and validation of our machine learning models. The systematic exploration of these phase spaces revealed numerous new potential superconductors with transition temperatures above 20K.

ICAMS

Department Computational Design of Functional Interfaces CoDeFi

8. Department Computational Design of Functional Interfaces

Group leader:
Prof. Dr. Silvana Botti

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Dr. Preeti Bhumla
Xiao Chen
Kun Gao
Jinyin Huang
Nico Kawashima
Martin Keller
Dr. Michael Seifert
Preeti Sharma
Dewen Sun

► Research

Research at the Department of Computational Design of Functional Interfaces combines advanced ab initio simulation techniques with experimental collaborations to investigate electronic excitations in complex materials. Through computational materials modelling, we optimize existing materials and discover new ones, exploring heterostructures, defects, alloys, and doped crystals, thus bridging condensed matter physics, materials chemistry, and computer science.

Currently, our primary research efforts concentrate on two key areas: designing functional interfaces and developing high-throughput methods for doping and alloy engineering of semiconductors. These efforts directly address global energy challenges and contribute to the transition to green energy by developing improved materials for technologies ranging from solar cells and batteries to photocatalysts and low-power devices. As area leader for "Theory and Computation" within the NFDI consortium FAIRmat, we also contribute to building a FAIR data infrastructure for condensed matter physics, ensuring our research supports a sustainable scientific ecosystem.

► Competences

Our group possesses deep expertise in the theoretical and computational investigation of electronic properties in functional materials. We specialize in first-principles methodologies based on density functional theory (DFT) and incorporate advanced many-body theories to achieve accurate and predictive results. A key strength is our focus on theoretical spectroscopy, enabling us to simulate in real-time the material's response to external stimuli, such as electromagnetic radiation, and compare directly with experiments.

Beyond these core competencies, we work on the development of new approximations for DFT and time-dependent DFT, and we have pioneered the integration of machine learning with DFT to accelerate the discovery of novel functional materials with enhanced electronic properties. We conduct high-throughput computational studies to identify effective doping strategies and discover promising alloys for energy-related applications. Furthermore, we have developed and applied constrained structure prediction methods to investigate nanostructured materials and interfaces.

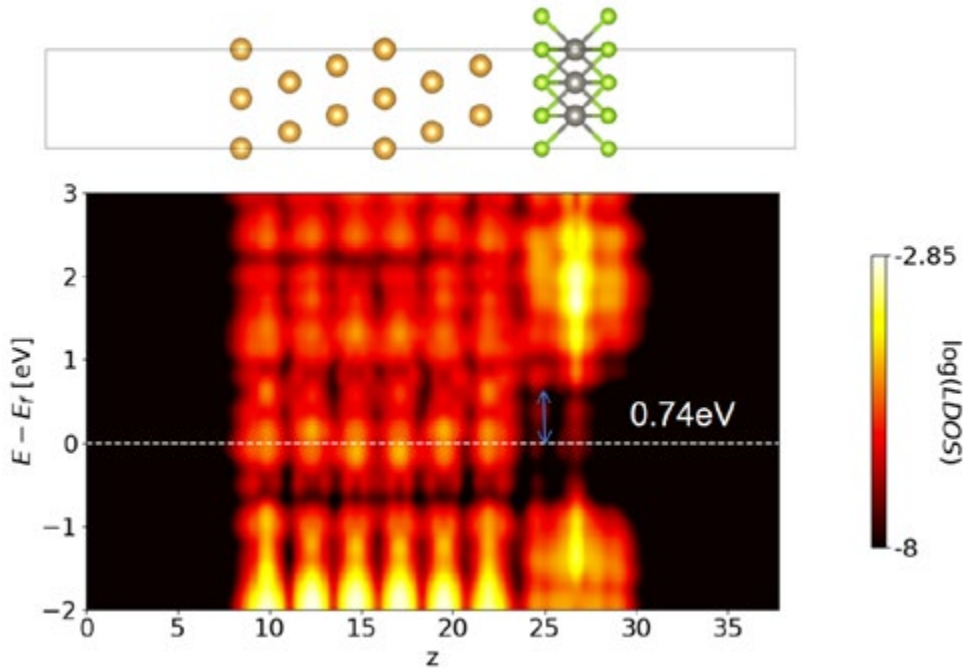

Fig. 8.1: Example of calculation of band diagram using the local density of states. The colour plot shows the local density of electronic states of a monolayer of WSe_2 on a gold substrate at energy E (having set to zero the Fermi energy E_F) along the axis z perpendicular to the interface. In the top panel the atomic structure along the same axis z is depicted: gold atoms are orange, tungsten atoms are grey and selenium atoms are green. The Schottky barrier, controlled by the Fermi level pinning, has a height of 0.74 eV.

Predicting electronic properties of functional interfaces

Understanding electronic excitations at functional interfaces is crucial for advancing electronic devices. Our group develops and applies computational materials modelling to create enhanced electronic and quantum materials through heterostructure design. Addressing the challenge of accurately calculating complex interfaces, we have developed density functionals for interfaces and 2D material properties, achieving accuracy comparable to more computationally intensive methods. For example, we investigated strontium germanate (SGO) on silicon (Si) as a photocathode, confirming a type-III band alignment suitable for photocatalytic water splitting. Currently, the group collaborates on projects involving diverse interfaces, compiling data into a database of interface band diagrams. Future efforts will employ AI to analyse this data, building predictive models for interface design and identifying key structural and chemical characteristics for specific functionalities.

T. Rauch, P. Marton, S. Botti, and J. Hlinka,
Band alignment at the strontium germanate interface with silicon,
Phys. Rev. B 107, 115303, 2023

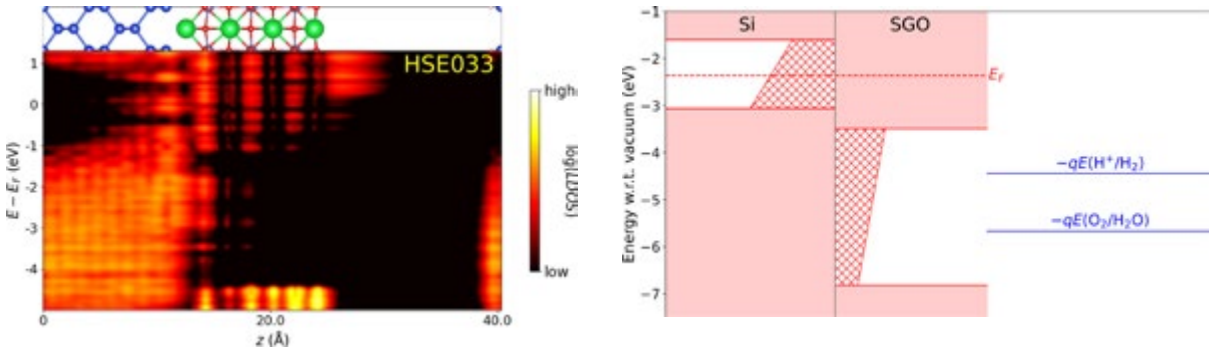

Fig. 8.2: Left panel: Atomic structure and local density of electronic states of SGO on a Si substrate, calculated with a modified hybrid density functional. Right panel: Schematic representation of the band edges of the SGO/Si system extracted from the local density of states, plotted together with the redox potentials of water splitting reactions.

Optimizing copper iodide-based transparent semiconductors

Transparent electronic components are essential for future technologies like transparent electrodes and solar windows. While n-type transparent conducting materials (TCMs) are well-established, high-performing p-type TCMs are lacking, hindering the creation of transparent p-n junctions. CuI is a promising p-type TCM, but its hole conductivity needs improvement. Our group, within the DFG research unit "CuI as multifunctional semiconductor" and in collaboration with experimental partners, uses high-throughput density functional theory calculations to explore doping and alloying strategies for CuI. Previous work demonstrated the effectiveness of chalcogen doping (S, Se) to increase hole concentration. Recently, we predicted that ternary Cu-I-S/Se compounds offer even greater control. Using the minima hopping method for crystal structure prediction, we explored these ternary phase diagrams, identifying 11 stable crystalline structures (9 unreported), including promising p-type TCMs and metallic topological semimetals. These TCMs exhibit strong p-d hybridization for high hole mobility and tuneable hole concentration. Current experimental efforts aim to synthesize and characterize these predicted compounds for integration into transparent devices.

M. Seifert, T. Rauch, M.A.L. Marques, and S. Botti, Computational prediction and characterization of CuI-based ternary p-type transparent conductors, J. Mater. Chem. C 12, 8320-8333, 2024

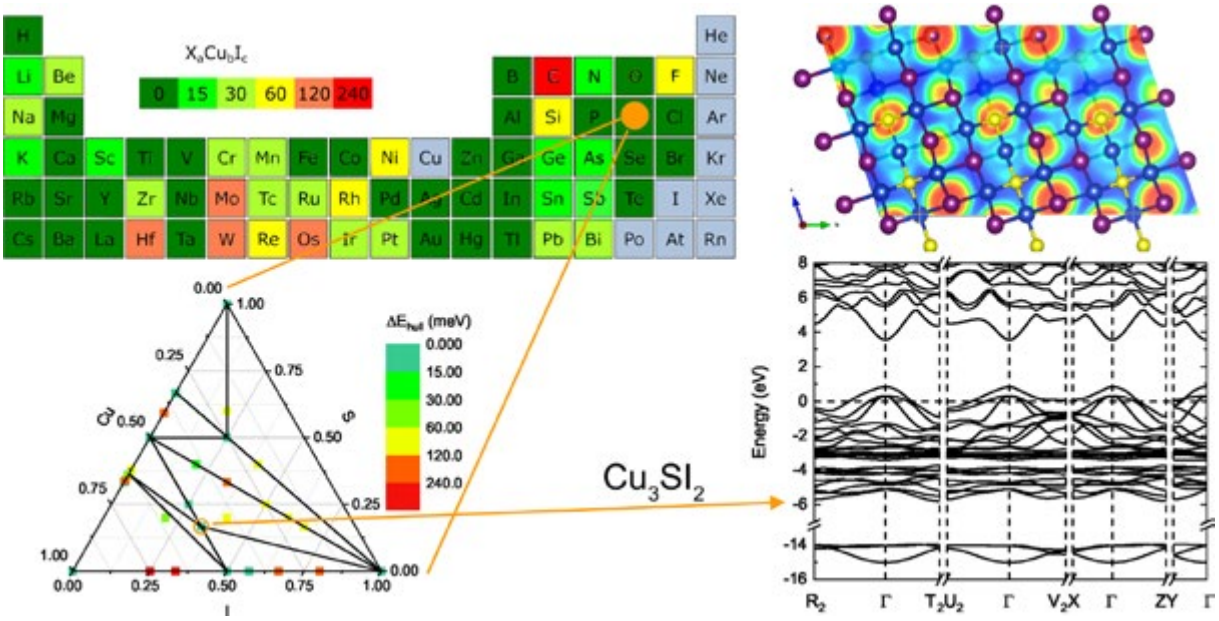

Fig. 8.3: The ternary phase diagram of Cu-S-I is shown as an example (bottom left). The colour indicates the distance from the convex hull of stability of the corresponding compounds (i.e., red is unstable and green is stable). On the right side of the figure the crystal structure of Cu_3SI_2 (top right) with a superposed electron localization function and the electronic band structures of Cu_3SI_2 (bottom right) are shown.

ICAMS

Scale-Bridging Simulation of Functional Composites SFC

9. Scale-Bridging Simulation of Functional Composites

Group leader:
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Group members:
Lan-Tien Hsu
Susanne Kunzmann
Mauwa Namisi
Benyao Sun

► Research

The group's goal is to design ferroelectric materials and composites as well as materials with displacive phase transitions, with superior functional properties. The main focus is on perovskites (ABO_3, or $A'BX_3$ with A:alkali earth metals, A': molecules, B: transition metals and X: halide ions), which are widely used in various applications and are promising for future efficient solid-state cooling devices based on the electrocaloric effect. Our approach to contribute to the fundamental understanding and the nano-scale control of the material's response to external stimuli (elastic, optical, electric) is the scale-bridging optimization of the internal structure, combining the benefits of substitution and doping, defects of different type and dimensions, domain wall engineering and interface design in composites. 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 and density functional theory simulations
- Ferroic materials and composites
- Functional (piezoelectric, dielectric, caloric, magnetic) responses
- Displacive phase transitions

One research focus in 2023/2024 was on ferroelectric domain walls. Particularly, we looked at the microscopic processes governing the domain wall dynamics driven by external electrical fields in orthorhombic ferroelectric phases and analyzed the electrocaloric response related to 180° domain walls.

A second focus was on displacive phase transitions, unifying common motives across disparate material classes, and focusing in more detail on metastable phases, transition paths and substitution in $Nb_{1-x}Ta_x$ as well as on the direction dependency of the phase diagramme of $BaTiO_3$ in an external field. Third, we worked on the impact of defect dipoles and point defects on phase stability and domain wall motion.

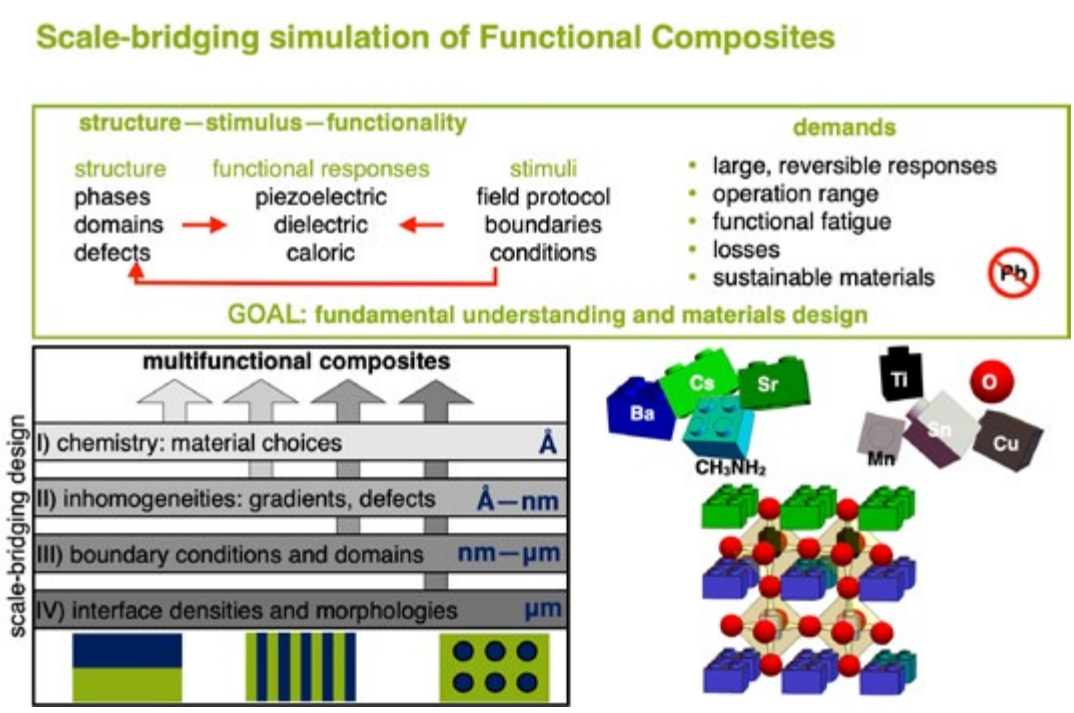

Fig. 9.1: Scale-bridging simulation of Functional Composites

Ab initio modelling of the Electrocaloric effect

The electrocaloric effect is the adiabatic temperature change induced by the change of an applied external field. This temperature change is maximal if the field induces a first-order phase transition and only moderate within one ferroelectric phase. Thus, either temperature and reversibility of the phase transition, or the response in one phase have to be optimized to reach stable and efficient cooling at any temperature of interest.

We first analyze the full temperature field-direction phase diagramme of BaTiO3 including the direction dependency of thermal hysteresis and caloric response. While the inverse caloric response at the lower phase transitions is neither reversible for moderate field strengths nor robust against misaligned fields, a large conventional caloric response is possible in a broad range of directions at the two transitions at higher temperatures. This also allows for large responses in textured polycrystals. Second, we dispel the common misconception that domain walls generally improve the caloric response in one phase and show that the responses of static 180° domains compensate each other, while the field-induced wall motion even heats up the material irreversibly contradicting cooling applications.

L.T. Hsu, F. Wendler, and A. Grünebohm,
Electric field direction dependence of the electrocaloric effect in $BaTiO_3$,
Phys. Rev. Mat., 8, 094408, 2024

A. Grünebohm, S.-H. Teng, and M. Marathe,
Influence of domain walls and defects on the electrocaloric effect,
J. Phys. Energy, 5, 034010 202

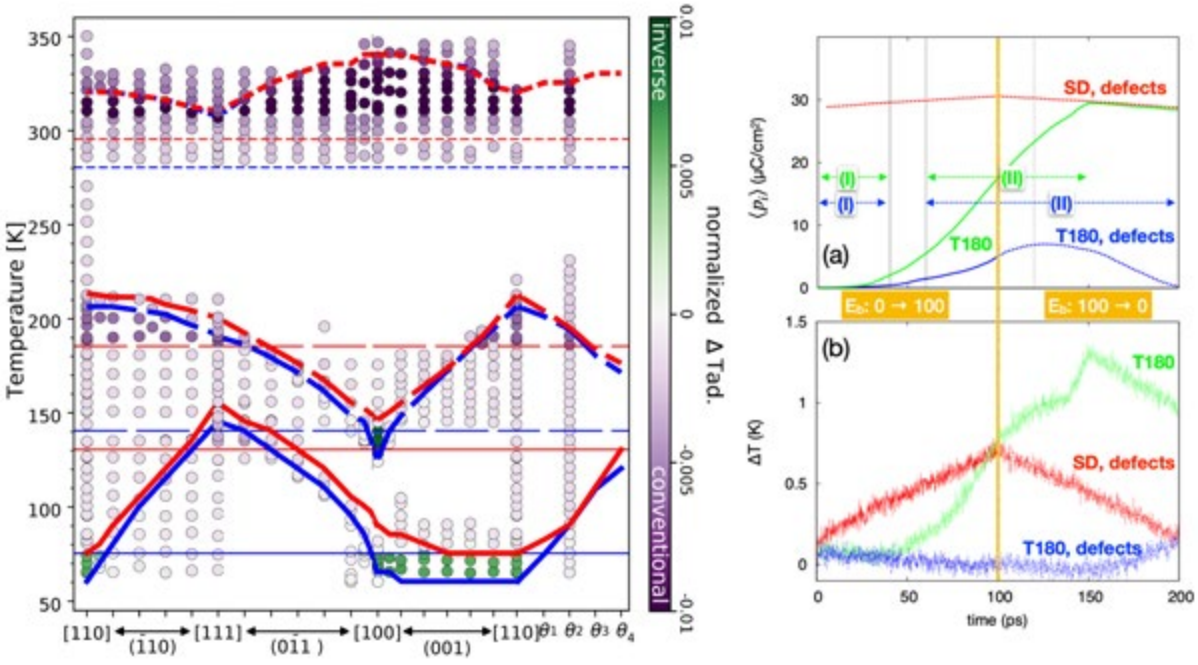

Fig. 9.2: Left: Temperature-electric field direction phase diagramme of $BaTiO_3$ with transition temperatures predicted in cooling (blue lines) and heating (red lines) simulations and normalized caloric response $\Delta T/T_{in}$ (color encoding of dots) depending on field direction and initial temperature T_{in}. Right: Caloric response of the tetragonal phase (initial temperature T_{in}: 260 K) for ramping on and off an external field along a [100]-type direction (E_b). Systems with: 180° domain walls (green), 1% defect dipoles (red), and both, walls and defects (blue), are compared for field intervals (I) pinned walls and (II) moving walls. In both cases for an external field strength of 100 kV/cm.

Displacive phase transitions in complex solids

Several classes of materials, ranging from simple metals to complex intermetallics and even to insulating materials, manifest displacive phase transitions related to similar electronic and phononic instabilities in conjunction with similar specific microstructural features. These transitions are associated with a wide range of fascinating properties and functionalities, which are studied in disparate communities. We aim at a unified framework for understanding and designing these transitions in all material classes.

As example, we revisit the well-characterized material Nb, which surprisingly shows not yet understood anomalies. We combine the analysis of phonon spectra, transition paths and formation energies, and include the fact that Nb crystals are usually contaminated with Ta into our study. One important outcome is that Ta substitution lowers the energy of the σ-phase, which is as low in energy as the bcc phase for pure Ta.

A. Grünebohm, A. Hütten, A. E. Böhmer, J. Frenzel, I. Eremin, R. Drautz, I. Ennen, L. Caron, T. Kuschel, F. Lechermann, D. Anselmetti, T. Dahm, F. Weber, K. Rossnagel, G. Schierning,
A unifying perspective of common motifs that occur across disparate classes of materials harboring displacive phase transitions,
Adv. Energy Mater., 13, 2300754, 2023 (a)-(c)

S. Kunzmann, T. Hammerschmidt, G. Schierning, A. Grünebohm,
Ab initio study of transition paths between (meta) stable phases of Nb and Ta-substitued Nb,
Phys Rev Mater 8, 033603, 2024 (d)-(f)

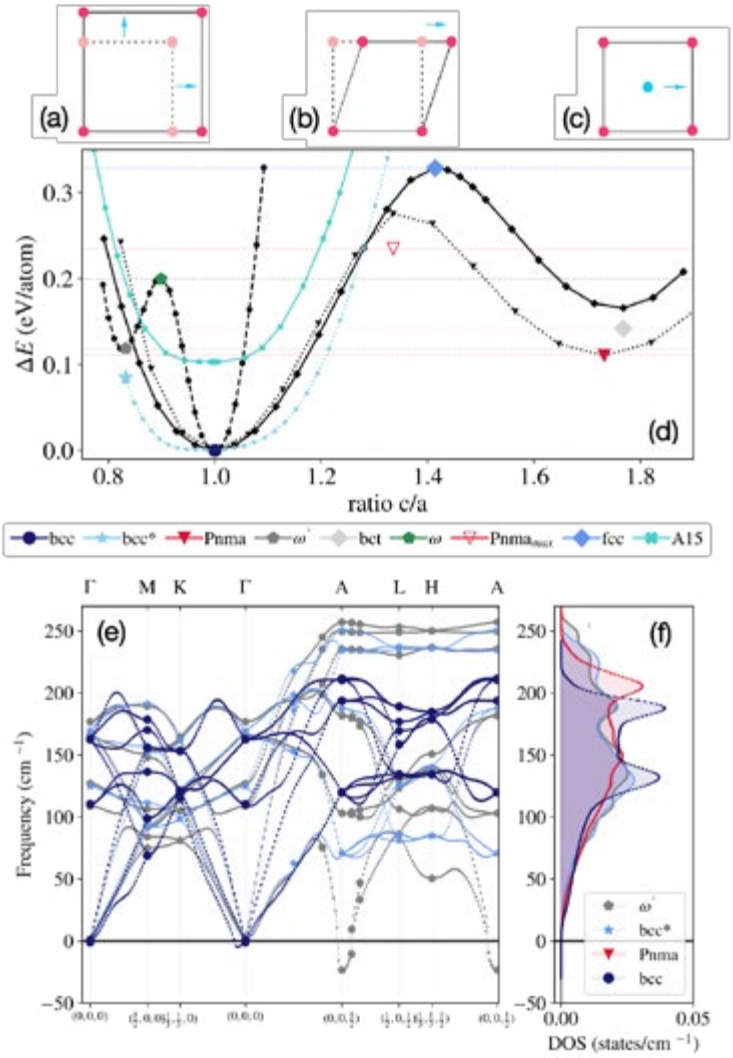

Fig. 9.3: (a)-(c) Prototypes of displacive phase transitions: (a) volume changes (b) shearing (c) atomic displacements. (d)-(f) Results for Nb: (d) Energy landscape for the deformation of the cubic bcc structure of Nb to various meta-stable structural phases and underlying phonon (d) spectra and (f) densities of states.

Domain wall motion in orthorhombic ferroelectrics

Ultradense domain walls are increasingly important for many devices, but their microscopic properties are so far not fully understood, and most microscopic studies are restricted to tetragonal ferroelectrics. Here, we combine molecular dynamic simulations with an analysis of cluster distributions to study the field-induced domain wall motion in the orthorhombic phase of the prototypical ferroelectric $BaTiO_3$. We show that in this phase 180° domain walls move by multistep 90° degree switching. While it has been reported before that the energy barrier for 90° switching may be smaller than the one for direct 180° switching, it was so far believed that only complex coherent switching processes can realize this. We show that a local realization of 90° degree switching with complex transient dipole patterns is possible on the moving domain wall.

R. Khachaturyan, Y. Yang, S.-H. Teng, B. Udofia, M. Stricker and A. Grünebohm,
Microscopic insights on field-induced switching and domain wall motion in orthorhombic ferroectrics,
Phys Rev Mater. 8, 024403, 2024

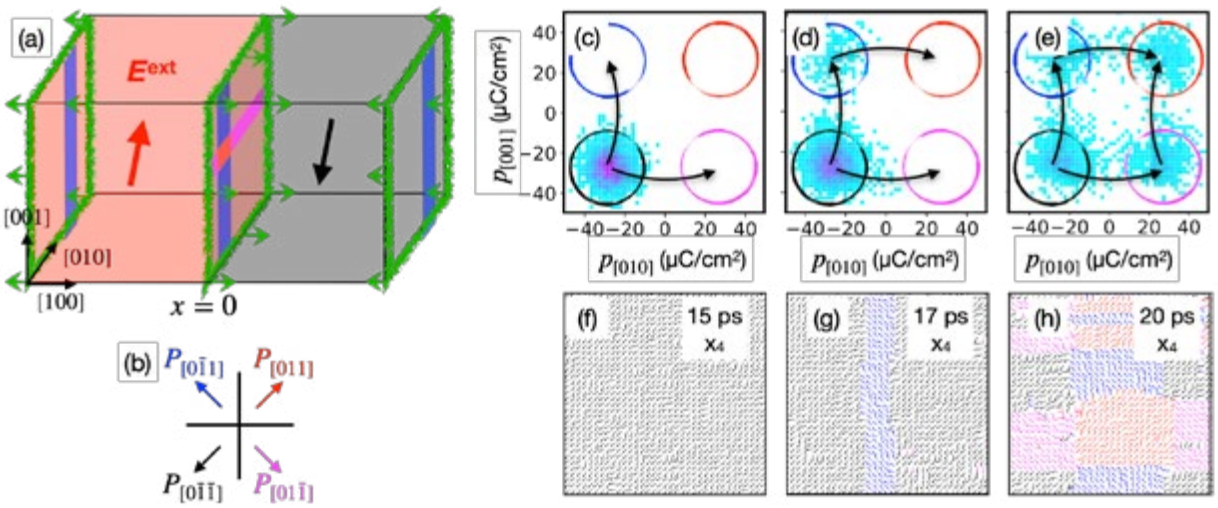

Fig. 9.4: Multistep polarization switching in orthorhombic $BaTiO_3$: (a) Illustration of the simulation setup with 180° domain walls normal to [100] (green frames). The local polarization in both domains points along ±P[011]. (b) Color encoding of the four polarization directions on the domain wall plane. (c)-(h) time-evolution on a plane in the negative domain in (c)-(e) polarization (f)-(h) and real space. (a)/(d) 15 ps, (b)/(e) 17 ps and (e)/(f) 20 ps after the field has been applied along [011]. Domains with P[01-1] and P[0-11] polarization nucleate and grow and if they cross the polarization switches to the final direction.

ICAMS

Materials Informatics and Data Science MIDS

10. Materials Informatics and Data Science

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

Group members:
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Gauravkumar Lathiya
Behnam Mardani
Doaa Mohamed
Benjamin Udofia
Lei Zhang
Qi Zhang
(starting March 2025: Swetha Pemma)

▸ Research

The increasing number of available materials data and the ongoing effort in the Materials Science community to efficiently collect, curate, and manage multidimensional heterogeneous research data forms the basis for the research in the Materials Informatics and Data Science group. The group's main target is the efficient navigation and exploration of materials data space through the development and implementation of interpretable, robust, controllable and generalizable tools. Our research is situated at the intersection of materials science, physics, chemistry, and data science which is reflected in the three areas: plasticity, AI & materials, and collaborations.

Our research in plasticity involves creating representative datasets of dislocation trajectories using discrete dislocation dynamics. We apply manifold learning techniques to develop new representations of these complex systems. These datasets also help to map simulated and experimentally-obtained diffraction patterns, thereby improving the experimental characterization of dislocations and their interactions with defects. This area has been strengthened by the ERC Starting Grant DISCO-DATA since November 2024.

In the AI & materials domain, we focus on multimodal document mining. By developing methods that use word embeddings, we explore materials space and create computationally efficient surrogate models to predict composition-property correlations based solely on text data. Additionally, we engage in 'post-publication research data management' of largely experimental results by using Large Language Models to create structured datasets from unstructured journal articles, extract and classify figures, and digitize tabular data. In addition, we are involved in two projects within the Collaborative Research Center 'Atomic-scale understanding and design of multifunctional compositionally complex solid solution surfaces'. One project focuses on FAIR data management solutions for heterogeneous materials data, while the other develops tools to fuse this data to address optimization tasks in the consortium. We also contribute the project 'Multimodal multiscale correlative microscopy of reduction processes' within the International Max Planck Research School Sustainable Metallurgy, aiming for a scale-bridging understanding of hydrogen-based iron ore reduction.

Further research includes atom-scale analysis of grain boundary structures, prediction and optimization of synthesis parameters for mechanochemistry, and Deep Learning-based segmentation of high-entropy alloy microstructures.

► Competences

- Knowledge extraction and text mining
- Atomistic and mesoscale simulation of mechanical properties
- Full-stack data-driven model development: Dimensionality reduction, clustering, estimators, active learning
- Heterogeneous materials data management and mining

Mining latent knowledge in text

Scientific articles contain hidden, so-called latent knowledge which can be extracted through text mining approaches. One variant of text mining is the creation of word embeddings through a method called word2vec. Embeddings are created by training a small neural network on a corpus. The resulting numerical values capture correlations between words. We have developed and end-to-end solution for the creation of such embeddings which includes API access to publishers to retrieve abstracts, preprocessing of raw text, and subsequent model fitting. We used these word embeddings then to predict composition-property correlations for thin-film composition spread materials libraries. Specifically, we predict correlations with resistance, dielectric properties, and reaction-specific electrocatalytic behavior to guide the development, discovery, and optimization of compositionally complex solid solutions as novel catalysts.

L. Zhang, M. Stricker,
MatNexus: A comprehensive text mining and analysis suite for materials discovery
SoftwareX, 26, 101654, 2024, https://doi.org/10.1016/j.softx.2024.101654

Unnamed: 0	abstract
0	absorption dominant shielding material propose magnetic material work frequen...
1	actively study lead free antiferroelectric afe material nanbo3 na nb o long s...
2	thereinto design new electrocatalyst high activity selectivity draw inspirati...
3	accord experimental result growth evolution oxide film divide three stage sta...
4	nevertheless lack general method pattern multiple metal pose limit develop dn...
5	first analyze limitation bring small datum workflow material machine learning...
6	report discovery metallic compound tifexcu2x−1sb ti fex cu sb tife1.33sb ti f...
7	major challenge material scientist metallurgist stage predict crystal structu...
8	benefit metallic level conductivity large adjustable gallery space low ion di...
9	implement model enable study topography groove profile scratch force residual...

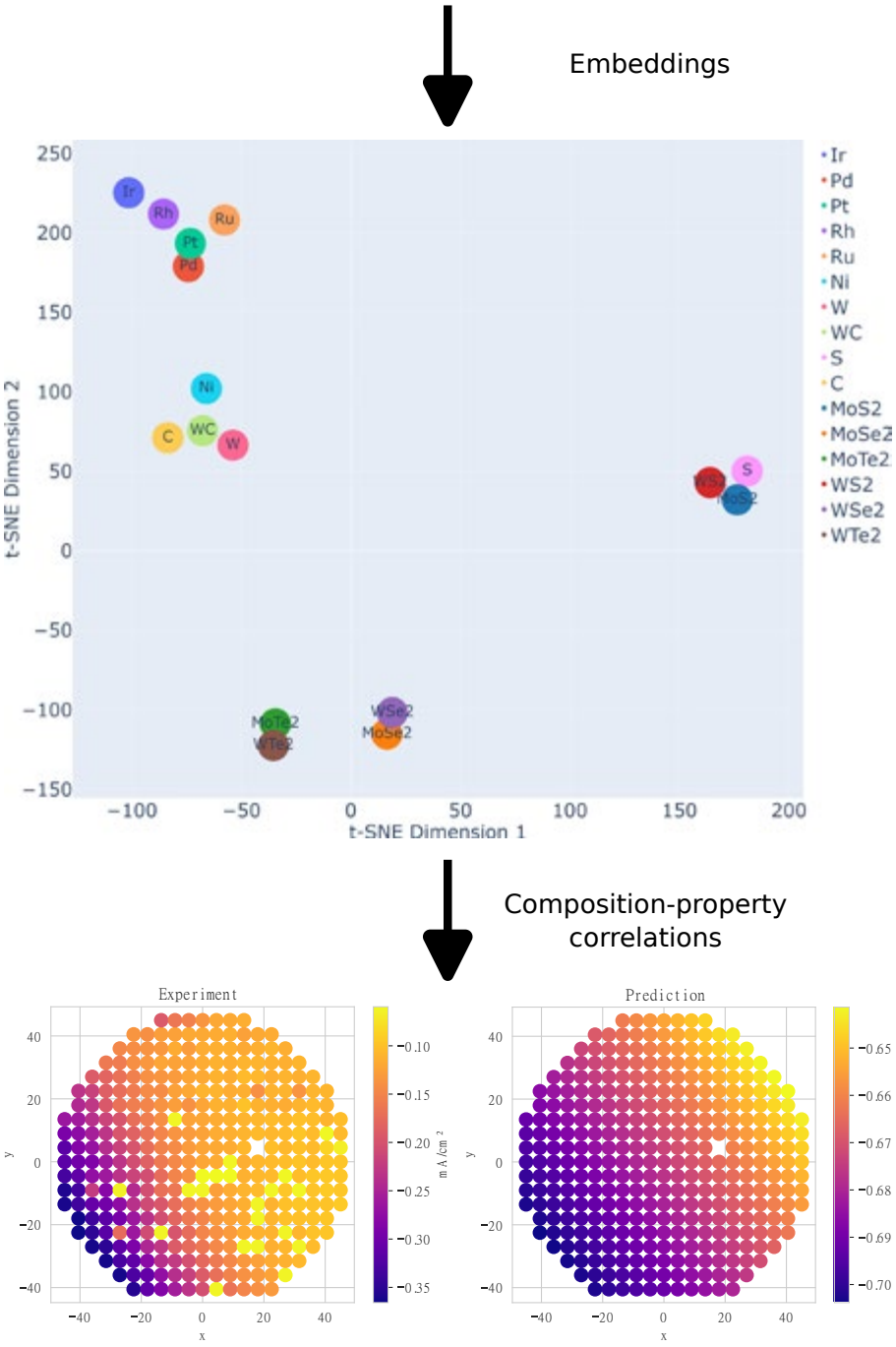

Fig. 10.1: A corpus of relevant open source abstracts is collected (top) and used for the creation of word embeddings. Embeddings capture the relationship between words, which also includes materials. High-dimensional numerical representations of words can be used to create a dimensionality-reduced map (center) of the relationship between materials. We use such embeddings to predict composition-property relationships for materials discovery (bottom), which correlate very well with experimental measurements.

Improving existing experimental characterization techniques using data science

Orientation mapping of materials surfaces is typically done using Electron Backscatter Diffraction (EBSD). Each Kikuchi pattern is assigned a single crystallographic orientation. In regions of the crystal where defects like (small angle) grain boundaries are present, a Kikuchi pattern contains signals from two crystallographic orientations. By using constrained non-negative matrix factorization, we showed that such a superposed signal of two crystallographic orientations can be factorized and the respective weights of the contributing signals can be recovered. This allows a sub-measurement-area resolution of the detection of defects down to below 1 degree of difference between the superposed orientation signals. Our method is computationally cheap but provides a similar segmentation as the much more expensive Rotation Vector-based EBSD with minimal user input. Future applications beyond orientation segmentation will be phase segmentation for the intermediate phases in hydrogen-based iron ore reduction.

A. Chauniyal, P. Thome, M. Stricker,
Employing Constrained Nonnegative Matrix Factorization for Microstructure Segmentation,
Microscopy and Microanalysis, 2024, ozae056, https://doi.org/10.1093/mam/ozae056

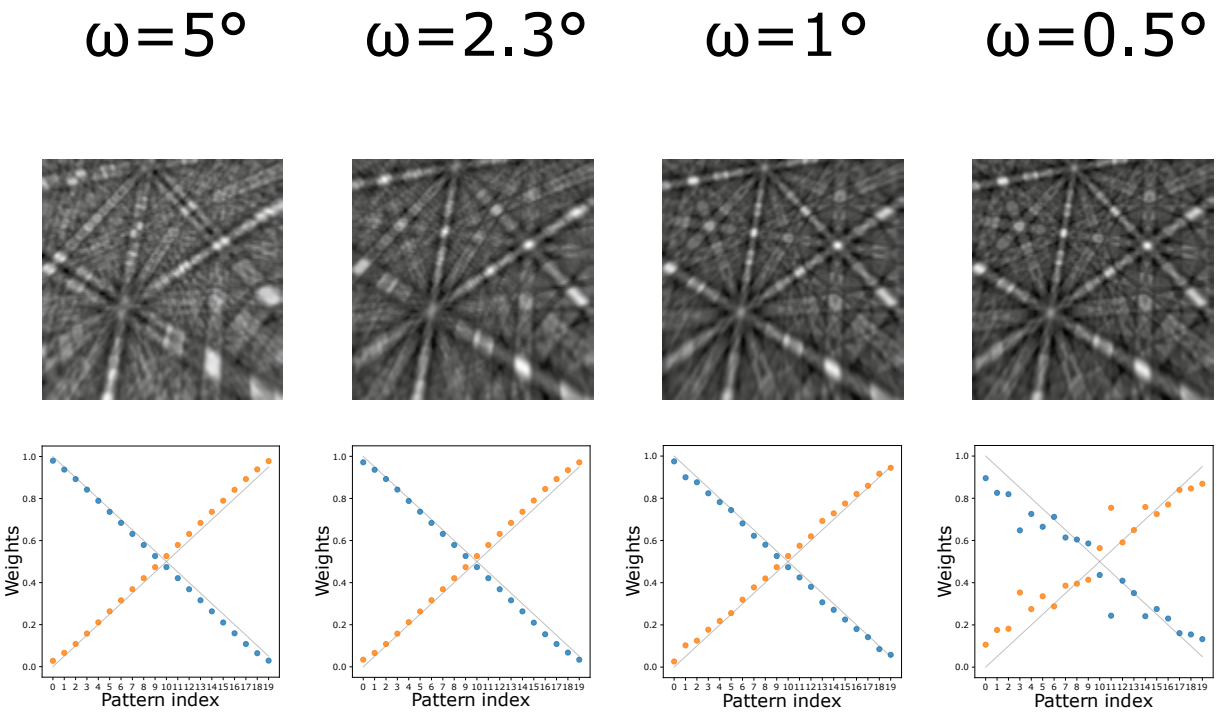

Fig. 10.2: Resolution limit test for constrained non-negative matrix factorization of simulated Kikuchi patterns with 20 different mixing ratios: Seemingly blurry overlapping signals (1 degree) can still be clearly factorized into their 2 components including their respective weights.

Dislocation structure representations

Dislocation structures are typically complex networks of connected lines. These are notoriously difficult to characterize and analyze beyond measures of densities and curvatures. A meaningful representation, however, is the basis for modeling such systems at longer length and time scales. These do not exist yet. By employing manifold learning techniques on spatially resolved dislocation density fields of simulated dislocation structures, we presented a first step towards a formalization of the development of such representations for dislocation networks. The resulting maps are physically interpretable and encode the relationship between individual data points: increasing strain results in a divergence between different simulated trajectories; different sectors of the map correlate with the crystallographic compression direction. Next steps in this direction are the inclusion of graph measures together with the density field to encode connectivity of dislocation networks.

B. Udofia, T. Jogi, M. Stricker,
Dislocation cartography: Representations and unsupervised classification of dislocation networks with unique fingerprints APL Machine Learning,
3, 016103, 2025, https://doi.org/10.1063/5.0224710

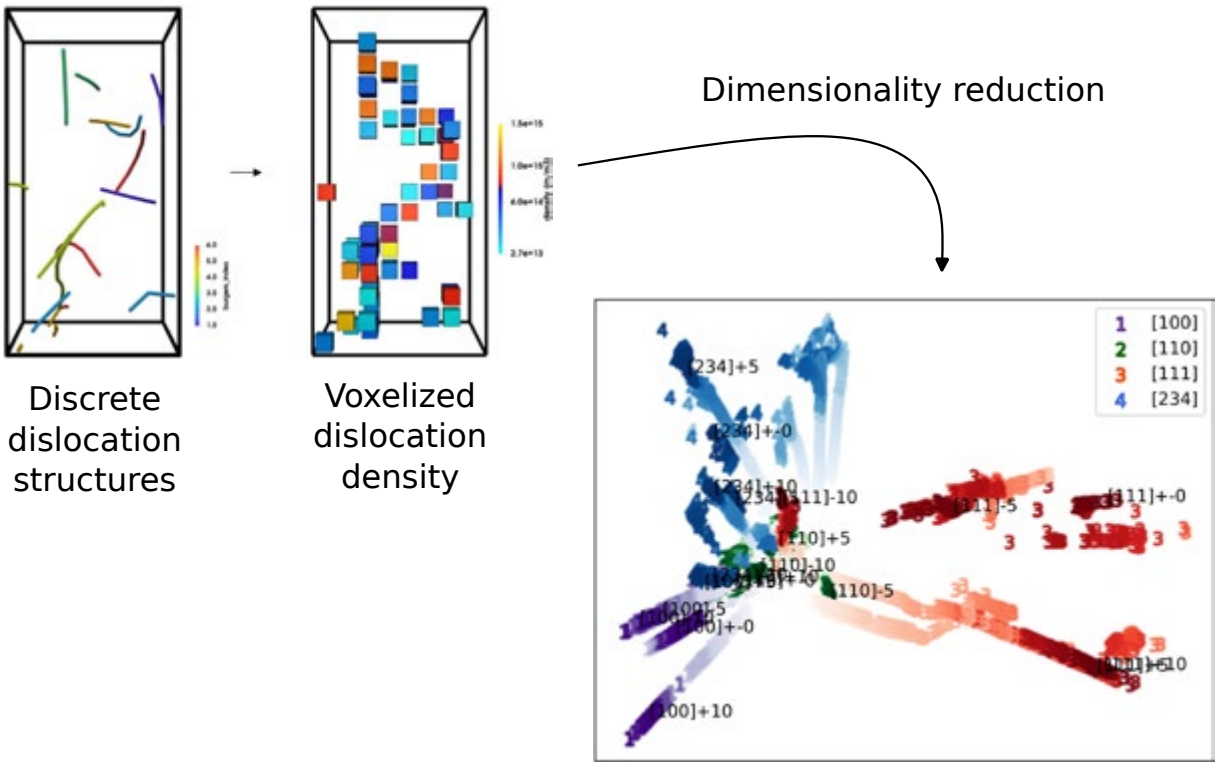

Fig. 10.3: Simulated discrete dislocation dynamics trajectories (left) are converted to 3D dislocation density fields (center) with 1024 dimensions. This representation is then used in an Isomap manifold learning algorithm and projected into 2D (right). Colors indicate the crystallographic compression direction; slight deviations from a perfect orientation are individually marked. Faint to dark coloring correlates with total strain: the darker the color, the larger the plastic compressive strain.

ICAMS

High-Performance Computing in Materials Science

HPC

11. High-Performance Computing Materials Science

Group leader:
Prof. Dr. Godehard Sutmann

Group members:
David Immel

▸ 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 in international communities. Currently, one focus is given to a new approach for an adaptive coupling of interaction potentials, performance portability of codes between different computer architectures, 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 collaboration with the Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich and the CECAM community.

▸ Competences

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

Spatially adaptive hybrid interaction potentials for large scale simulations

Large-scale atomistic simulations rely on interatomic potentials, providing an efficient representation of atomic energies and forces. Modern machine-learning (ML) potentials provide the most precise representation compared to electronic structure calculations, while traditional potentials provide a less precise but computationally much faster representation and, thus, allow simulations of larger systems. A new method has been developed to combine both a traditional and an ML potential into a multi-resolution description, leading to an adaptive-precision potential with an optimum of performance and precision in large, complex atomistic systems. The required precision is determined per atom by a local structure analysis and updated automatically during simulation. Copper has been used as a demonstrator material with an embedded atom model as classical force field and an atomic cluster expansion (ACE) as ML potential, but, in principle, a broader class of potential combinations can be coupled by this method. The approach is developed for the molecular-dynamics simulator LAMMPS and includes a load-balancer to prevent problems due to the atom-dependent force-calculation times, which makes it suitable for large-scale atomistic simulations. The developed adaptive-precision copper potential represents the ACE forces with a precision of 10 meV/Å and the ACE energy exactly for the precisely calculated atoms in a nanoindentation of 4×10^6 atoms calculated for 100 ps, and shows a speedup of more than 10 compared with a full ACE simulation.

Parallel hybrid Monte Carlo / molecular statics for simulation of solute segregation in solids

A parallel hybrid Monte Carlo / molecular statics method has been developed for studying segregation of interstitial atoms in the solid state. The method is based on the efficient use of virtual atoms as placeholders to find energetically favorable sites for interstitials in a distorted environment. MC trial moves perform an exchange between a randomly chosen virtual atom with a carbon atom followed by a short energy minimization via MS to relax the lattice distortion. The proposed hybrid method is capable of modeling solute segregation in deformed crystalline metallic materials with a moderate MC efficiency. To further improve the sampling of configuration space, a prediction scheme is developed, which allows a first estimate whether the insertion or removal of a particle from the atomistic system will lead to an energy reduction or an increase. A multipole-based scheme is used, which characterizes the short-range environment of an insertion/removal particle and compares coefficients with database entries from historical data (on-the-fly training data set). The success prediction for particle insertion is a fast procedure and can save a large amount of CPU time.

Performance portability between computer architectures

Each hardware vendor has its own preferred model for programming GPUs. To enable the transition between different types of computer architectures, different programming models exist, part of which also claim performance portability. The N-body problem has been implemented as a benchmark system for using portable programming frameworks and APIs preferred by the vendors. The performance of the portable solutions has been compared to the performance of the native solution on each hardware both in absolute numbers and as fraction of the achievable peak performance. Overall best results could be obtained for Sycl, OpenMP and Kokkos. The latter is one of these frameworks, which will further be used together with the library Cabana for the extension of scalable electrostatics solvers, e.g. the P3M method. This method includes the usage of Fast Fourier transformations, which barely scale on large GPU partitions. Therefore, in future also hybrid partitions and improved FFT strategies for real and reciprocal space calculations will be considered.

Load balancing methods and library development

The load balancing library ALL, developed at JSC, has been adapted to the community MD code LAMMPS. An extension of the tensor decomposition method, using a cost function, which is based on a maximum work difference between domains, has been developed. It was shown that it is superior with respect to the classical tensor decomposition method. Due to a cartesian decomposition in spatial dimensions and conserving topology of the initial decomposition it is well-suited for codes with regular decomposition strategies. More involved methods like the staggered domain decomposition method have also been included into LAMMPS via ALL. In a first benchmark run, methods from ALL could show superior scaling properties compared to native methods from LAMMPS. Ongoing work also considers histogram methods, both on a local and global scale. the P3M method. This method includes the usage of Fast Fourier transformations, which barely scale on large GPU partitions. Therefore, in future also hybrid partitions and improved FFT strategies for real and reciprocal space calculations will be considered.

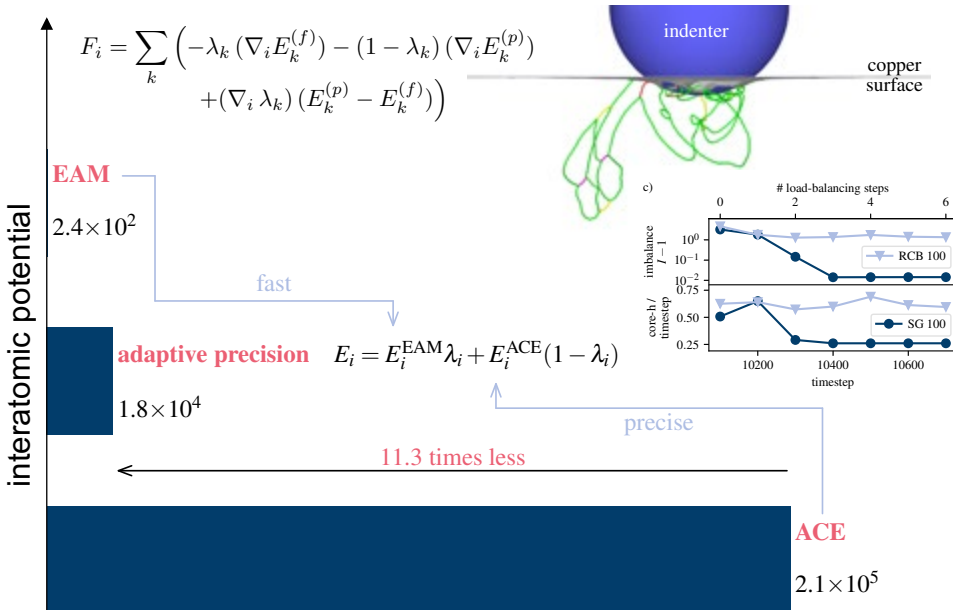

Fig. 11.1: Schematic summary of the spatially adaptive hybrid interaction potentials. For a demonstration, a copper system was used in the nano-indentation setup. Particle types are distinguished between types of potentials or their superposition according to a central-symmetry parameter. If the local structure of an atom is perturbed upon a threshold, a superposition between a classical EAM potential and an ACE potential is applied. For strong deviations, a full ACE is applied, which has a transition zone into the neighboring atom layers, where both ACE and EAM are superimposed. The developed algorithm is capable to conserve energy and momentum in the system if no external forces are applied.

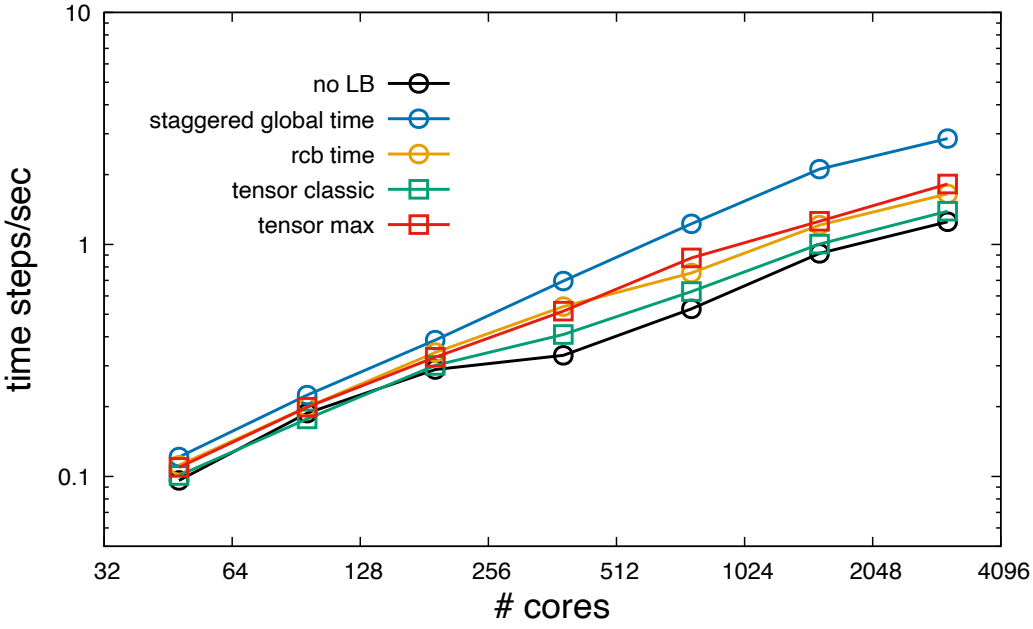

Fig. 11.2: Comparison of different load-balancing methods from the developed ALL library and the native implementations in the LAMMPS simulation code for the case of an adaptive precision interaction potential in the setup of a system with stocastically placed vacancies. The maximum tensor decomposition and staggered domain decomposition show both good scaling properties.

ICAMS

Publications

12. Publications

► Publications in Refereed Journals, Proceedings, and Books

A. Riyahi khorasgani, M. Younan, I. Steinbach, J. Kundin
Phase-field modeling of kinetics of diffusive phase transformation in compositionally-graded Ni-based superalloys
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M. Zheng, C. Zhao, X. Yan, R. Khachaturyan, F. Zhuo, Y. Huo, J. Koruza
Metal particle composite hardening in $Ba_{0.85}Ca_{0.15}Ti_{0.90}Zr_{0.10}O_3$ piezoceramics
Advanced Functional Materials
33, 2301356, 2023

A. Grünebohm, A. Hütten, A. E. Böhmer, J. Frenzel, I. Eremin, R. Drautz, I. Ennen, L. Caron, T. Kuschel, F. Lechermann, D. Anselmetti, T. Dahm, F. Weber, K. Rossnagel, G. Schierning
A unifying perspective of common motifs that occur across disparate classes of materials harboring displacive phase transitions
Advanced Energy Materials
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M. Keller, A. Belabbes, J. Furthmüller, F. Bechstedt, S. Botti
First-principles insight in structure-property relationships of hexagonal Si and Ge polytypes
Physical Review Materials
7, 064601, 2023

J. Schmidt, N. Hoffmann, H.-C. Weng, P. Borlido, P. J. M. A. Carriço, T. F. T. Cerqueira, S. Botti, M. A. Marques
Machine-learning-assisted determination of the global zero-temperature phase diagram of materials
Advanced Materials
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G. Eshlaghi, G. Egels, S. Benito, M. A. Stricker, S. Weber, A. Hartmaier
Three-dimensional microstructure reconstruction for two-phase materials from three orthogonal surface maps
Frontiers in Materials
10, 1–17, 2023

A. Nammalvar Raja Rajan, M. Krochmal, M. Shahmardani, T. Wegener, A. Hartmaier, T. Niendorf, G. Moeini
Micromechanical modeling of the low-cycle fatigue behavior of additively manufactured $AlSi_{10}Mg$
Materials Science and Engineering: A
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M. Azadi Tinat, M. Uddagiri, I. Steinbach, I. Lopez-Galilea
Numerical simulations to predict the melt pool dynamics and heat transfer during single-track laser melting of Ni-based superalloy (CMSX-4)
Metals
13, 1091, 2023

J. Kundin, I. Steinbach, S. Chakraborty
Phase-field simulation of texture evolution in magmatic rocks
JGR Solid Earth
128, 1–19, 2023

A. Grünebohm, S. Teng, M. Marathe
Influence of domain walls and defects on the electrocaloric effect
Journal of Physics: Energy
5, 034010, 2023

M. Shahmardani Firouzjah, R. Logvinov, T. Babinský, S. Guth, S. Paul, A. Biswas, N. Vajragupta, A. Hartmaier
Experimental assessment and micromechanical modeling of additively manufactured austenitic steels under cyclic loading
Advanced Engineering Materials
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H. Parida, J. Kundin, C. Alves
Study of the peritectic phase transformation kinetics with elastic effect in the Fe–C system by quantitative phase-field modeling
Computational Materials Science
224, 112160, 2023

J. Schmidt, H. Wang, G. Schmidt, M. A. Marques
Machine learning guided high-throughput search of non-oxide garnets
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S. Shanmugam, M. Peterlechner, M. Iskandar, U. Saikia, V. Kulitckii, M. Lipińska-Chwałek, J. Mayer, H. Rösner, T. Hickel, S. V. Divinski, G. Wilde
Coherent twin-oriented Al_3Sc-based precipitates in Al matrix
Scripta Materialia
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Phase-field study of the history-effect of remelted microstructures on nucleation during additive manufacturing of Ni-based superalloys
Metallurgical and Materials Transactions A
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A. Egorov, A. Subramanyam, Z. Yuan, R. Drautz, T. Hammerschmidt
Magnetic bond-order potential for iron-cobalt alloys
Physical Review Materials
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S. Starikov, D. Smirnova
Details of structure transformations in pure uranium and U-Mo alloys: Insights from classical atomistic simulation
Journal of Nuclear Materials
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S. Motahari, A. Chauniyal, R. Janisch
Investigating the microplastic behavior of hierarchical polycrystalline γ-TiAl microstructures
Computational Materials Science
226, 112197, 2023

A. Chauniyal, R. Janisch
How coherent and semi-coherent interfaces govern dislocation nucleation in lamellar TiAl alloys
Advanced Engineering Materials
25, 2300121, 2023

Y. Lysogorskiy, A. Bochkarev, M. Mrovec, R. Drautz
Active learning strategies for atomic cluster expansion models
Physical Review Materials
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N. Wang, T. Hammerschmidt, T. Hickel, J. Rogal, R. Drautz
Influence of spin fluctuations on structural phase transitions of iron
Physical Review B
107, 104108, 2023

T. Rauch, P. Marton, S. Botti, J. Hlinka
Band alignment at the strontium germanate interface with silicon
Physical Review B
107, 115303, 2023

E. Krüger, M. Seifert, V. Gottschalch, H. Krautscheid, C. Schnohr, S. Botti, M. Grundmann, C. Sturm
Optical properties of $Ag_xCu_{1-x}I$ alloy thin films
AIP Advances
13, 035117, 2023

Y. Jiang, M. A. Ali, I. Roslyakova, D. Bürger, G. Eggeler, I. Steinbach
3D phase-field simulations to machine-learn 3D information from 2D micrographs
Modelling and Simulation in Materials Science and Engineering
31, 035005, 2023

S. Benito, G. Egels, A. Hartmaier, S. Weber
Statistical characterization of segregation-driven inhomogeneities in metallic microstructures employing fast first-order variograms
Materials Today Communications
34, 105016, 2023

M. A. Ali, O. Shchyglo, M. A. Stricker, I. Steinbach
Coherency loss marking the onset of degradation in high temperature creep of superalloys: Phase-field simulation coupled to strain gradient crystal plasticity
Computational Materials Science
220, 112069, 2023

G. Cappellini, J. Furthmüller, F. Bechstedt, S. Botti
Electronic and optical properties of alkaline earth metal fluoride crystals with the inclusion of many-body effects: A comparative study on rutile MgF_2 and cubic SrF_2
Symmetry
15, 539, 2023

L. Zhao, J. Zhang, J. Zhang, H. Dai, A. Hartmaier, T. Sun
Numerical simulation of materials-oriented ultra-precision diamond cutting: Review and outlook
International Journal of Extreme Manufacturing
5, 022001, 2023

F. Pütz, N. Fehlemann, V. Göksu, M. Henrich, M. Könemann, S. Münstermann
A data driven computational microstructure analysis on the influence of martensite banding on damage in DP-steels
Computational Materials Science
218, 111903, 2023

A. Biswas, D. Kurtulan, T. Ngeru, A. Azócar Guzmán, S. Hanke, A. Hartmaier
Mechanical behavior of austenitic steel under multi-axial cyclic loading
Materials
16, 1367, 2023

A. Belabbes, S. Botti, F. Bechstedt
Erratum: Band lineup at hexagonal $Si_xGe_{1-x}/Si_yGe_{1-y}$ alloy interfaces
Physical Review B
107, 039903, 2023

P. Borlido, F. Bechstedt, S. Botti, C. Rödl
Ensemble averages of ab initio optical, transport, and thermoelectric properties of hexagonal Si_xGe_{1-x} alloys
Physical Review Materials
7, 014602, 2023

J. Hufert, A. Grebhardt, Y. Schneider, C. Bonten, S. Schmauder
Deformation behavior of 3D printed auxetic structures of thermoplastic polymers: PLA, PBAT, and blends
Polymers
15, 389, 2023

D. Gaertner, J. Kundin, I. Steinbach, S. V. Divinski, N. Esakkiraja, J. Berndt, A. Paul, A. Durand, G. Eggeler, J. Kottke, S. Klemme, G. Laplanche, G. Wilde
Tracer diffusion under a concentration gradient: A pathway for a consistent development of mobility databases in multicomponent alloys
Journal of Alloys and Compounds
930, 167301, 2023

M. Shahmardani Firouzjah, A. Hartmaier
Microstructure-sensitive crystal plasticity modeling for austenitic steel and nickel-based superalloy under isothermal fatigue loading
Metallurgical and Materials Transactions A
54, 1862–1873, 2023

▶ Bachelor, Master, and PhD Theses

M. Ali
High temperature creep in Ni-based superalloys
Ph.D. Thesis, Ruhr-Universität Bochum

M. M. Bruns
Simulating and characterizing cryogenic thermal cycling of a model glass former via molecular dynamics simulations
Ph.D. Thesis, Ruhr-Universität Bochum

A. Dimou
Phase diagrams and functional responses of ferroelectric solid solutions: An ab initio based molecular dynamics study
Ph.D. Thesis, Ruhr-Universität Bochum

A. Egorov
Atomistic simulation of iron-cobalt and niobium: From electrons to dislocations
Ph.D. Thesis, Ruhr-Universität Bochum

L. Huo
Microstructure evolution in polycrystals driven by magnetic fields: A multi-phase-field study
Ph.D. Thesis, Ruhr-Universität Bochum

Y. Liang
Atomistic transformations during nucleation and interface migration in metals
Ph.D. Thesis, Ruhr-Universität Bochum

P. Mathews
Ab-initio thermodynamics of defect phases
Ph.D. Thesis, Ruhr-Universität Bochum

I. Pietka
Atomistic simulation of partitioning in superalloys
Ph.D. Thesis, Ruhr-Universität Bochum

T. Pradhan
Atomistic simulations of hydrogen interactions with crystal defects in bcc-Fe
Ph.D. Thesis, Ruhr-Universität Bochum

A. Riyahi Khorasgani
Modeling diffusion phenomena in Complex Alloys: From multi-component diffusion to morphological instability of Kirkendall pores
Ph.D. Thesis, Ruhr-Universität Bochum

T. Schmalofski
Sampling of the multidimensional parameter space of grain boundary energies with atomistic simulations and statistical methods
Ph.D. Thesis, Ruhr-Universität Bochum

X. Song
Analysis and microstructure based simulation of fatigue damage in high-performance steels
Ph.D. Thesis, Ruhr-Universität Bochum

M. Uddagiri
Microstructure evolution during additive manufacturing of Ni-based superalloys
Ph.D. Thesis, Ruhr-Universität Bochum

S. Abbasimofrad
Characterization and deep-learning segmentation of microstructures in Fcc high entropy alloys
Master Thesis, Ruhr-Universität Bochum

A. Abbass
Atomistic simulation of grain boundary structural transformations in bcc metals
Master Thesis, Ruhr-Universität Bochum

Y. Bang
Chemical synthesis and characterization of nanostructured Ir/TiO_2
Master Thesis, Ruhr-Universität Bochum

H. U. Bhimavarapu
Modelling of adiabatic shear band initiation in polycrystals
Master Thesis, Ruhr-Universität Bochum

A. Chandramohan Vishvakarma
Impact of defect structures on Hydrogen diffusion in Nickel
Master Thesis, Ruhr-Universität Bochum

N. Farzaliyeva
Machine learning surrogate models for finite element simulations of the indentation process
Master Thesis, Ruhr-Universität Bochum

I. A. Garcia
A Comparison Analysis between Conventional and Machine Learning Model on Metal Plasticity
Master Thesis, Ruhr-Universität Bochum

M. Ghasemi
Microscopic insights on field induced switching and domain wall motion in ferroelectrics
Master Thesis, Ruhr-Universität Bochum

P. Gnanasivam
Grey-Box-Modellierung eines nichtlinearen Systems für die aktive, modellbasierte Schwingungsdämpfung
Master Thesis, Ruhr-Universität Bochum

P. Gordhandas Antala
Multiscale modelling of microstructure evolution under additive manufacturing conditions
Master Thesis, Ruhr-Universität Bochum

P.-Y. Huang
Molecular dynamic simulations of Si surfaces and growth
Master Thesis, Ruhr-Universität Bochum

C. L. Ihemaguba
Interdiffusion and martensitic transfomation in chemically complex shape memory alloys and selected sub-systems
Master Thesis, Ruhr-Universität Bochum

A. Jena
Calculating Indentation Schmid Factor (ISF) and analyzing complex stress state during nanoindentation using crystal plasticity
Master Thesis, Ruhr-Universität Bochum

Y. Jiang
Influence of free surface on cyclic plasticity and fatigue
Master Thesis, Ruhr-Universität Bochum

A. Karusala
Molecular dynamics simulations of dislocation–grain boundary interaction during nanoindentation of tungsten bi-cryst
Master Thesis, Ruhr-Universität Bochum

G. Lathiya
Yield stress prediction of dislocation structures using graph descriptors
Master Thesis, Ruhr-Universität Bochum

E. Mugabi
Investigation of the effects of grain orientation on the thermomechanical fatigue behavior of 316L stainlesssteel
Master Thesis, Ruhr-Universität Bochum

B. Mushtaq
Determination of residual stresses in turbo gear units
Master Thesis, Ruhr-Universität Bochum

S. R. Namireddy
Development, validation and comparision of atomic cluster expansion and ReaxFF inter-atomic potentials for Li-V-O terinary material system
Master Thesis, Ruhr-Universität Bochum

H. Nanayakkara
Numerical simulation of laser powder bed fusion additive manufacturing process of multicomponent Ni-based super alloys
Master Thesis, Ruhr-Universität Bochum

P. Nooshmehr
Training of machine learning models for the influence of porosity on the damage behavior of metals
Master Thesis, Ruhr-Universität Bochum

N. Ölcer
Ab initio simulation of solid solutions of $BaTiO_2$: The role of Ti substitution
Master Thesis, Ruhr-Universität Bochum

S. Prajapati
High current conductive adhesives
Master Thesis, Ruhr-Universität Bochum

N. Qi
Preparation and characterization of polymer membranes doped with ionic liquids for fuel cells
Master Thesis, Ruhr-Universität Bochum

Y. Rezek
Using machine learning surrogate models to determine material parameters by inverse analysis of indentation data
Master Thesis, Ruhr-Universität Bochum

S. Sarafrazian
Low pressure die casting of $AlSi_7Mg$ structural composite with AlMgSiCu insert: Production, Characterization and Simulation
Master Thesis, Ruhr-Universität Bochum

H. Sharma
Efficient fatigue modelling for large finite-element models
Master Thesis, Ruhr-Universität Bochum

A. Taheri Mofassal
Microstructure generation, modeling and fatigue analysis of friction-stir welded joint of an additively manufactured component and a cast component
Master Thesis, Ruhr-Universität Bochum

B. Udofia
Creating a catalog of dislocation microstructures expected in micromechanical experiments with descrete dislocation dynamics
Master Thesis, Ruhr-Universität Bochum

H. S. Wijekoon
Theoretical Investigation of <100> edge dislocations in ferroelectric perovskites
Master Thesis, Ruhr-Universität Bochum

M. Yang
Simulation of grain-structure formation in additive manufacturing process
Master Thesis, Ruhr-Universität Bochum

M. Younan
Effect of composition on high temperature creep of ERBO Ni-based superalloys
Master Thesis, Ruhr-Universität Bochum

ICAMS

Talks and Posters

13. Talks and Posters

▶ Invited Talks

10.01.2023
M. A. Stricker, L. Banko, N. Sarazin, N. Siemer, J. Neugebauer, A. Ludwig
Materials Informatics – appreciation of data and algorithms
Materials Data Science and Informatics (IAS-9), Jülich, Germany

28.02.2023
R. Drautz
Machine learning interatomic potentials for phase formation and phase diagrams
RESOLV, RUB, Germany

09.03.2023
R. Drautz
Atomic cluster expansion for learning the interaction between atoms
RESOLV Klausurtagung 2023, Harsewinkel, Germany

17.04.2023
M. A. Stricker, M. Ziemann, M. Walter, S. Weygand, P. Gruber, D. Weygand, A. Chauniyal, B. E. Udofia
Materials informatic for plasticity
DGM Fachausschuss Materials Modelling, Simulation, and Data, Aachen, Germany

18.04.2023
A. Grünebohm
Interplay of ferroelectric phase transitions domain structures and functional responses
784. WE-Heraeus-Seminar, Physikzentrum Bad Honnef, Germany

03.05.2023
R. Drautz
From electrons to the simulation of materials
Workshop: Complex Scientific Workflows at Extreme Computational Scales, IPAM, UCLA, Los Angeles, USA

09.05.2023
A. Grünebohm
Atomistische Simulationen zu ferroelektrischen Materialien
Forum Produktion, Österreichische Forschungsförderungsgesellschaft, Steyer, Austria

31.05.2023
A. Grünebohm, A. Dimou, R. Khachaturyan, S. Teng, M. Marathe, P. Hirel
Interplay of domain structure, phase transitions and functional responses in ferroelectric (Ba,Sr)TiO_3
Symposium: Materials for energy conversion systems: fundamentals, designs, and applications at the EMRS Fall Meeting, Strasbourg, France

14.06.2023
A. Grünebohm
Domain wall dynamcis in $BaTiO_3$ revisited
Ecole Central Lyon, Physique de la mati, France

29.06.2023
R. Drautz
ACE age: Applications, generalizations and extensions of the atomic cluster expansion
Los Alamos National Laboratory, USA

05.07.2023
R. Drautz
ACE age: Applications, generalizations and extensions of the atomic cluster expansion
Sandia National Laboratories, Albuquerque, USA

06.07.2023
F. Varnik
Solvent effects in shape memory polymers: Experiments and computer simulations
6th International Conference on Smart Materials and Spectroscopy, Monastir, Tunisia

17.07.2023
R. Drautz
Extending atomic interaction models
Virtual workshop Machine Learning Potentials - Status and Future (MLP-SAFE), Online

20.07.2023
R. Drautz
ACE age: Applications, generalizations and extensions of the atomic cluster expansion
Northwestern University, Evanston, Chicago, USA

17.08.2023
R. Drautz
ACE age: Applications, generalizations and extensions of the atomic cluster expansion
MPI für Eisenforschung, Düsseldorf, Germany

25.09.2023
R. Drautz
Atomic cluster expansion for a unified approach to machine learning potentials
TACO-NanoCat Conference, Vienna, Austria

10.10.2023
R. Drautz
From high-throughput DFT to the simulation of materials with the Atomic Cluster Expansion
Materials Design Users' Group Meeting, Vienna, Austria

24.11.2023
A. Grünebohm
Domain wall dynamcis in $BaTiO_3$ revisited
Theory seminar, University of Duisburg-Essen, Germany

22.01.2024
M. A. Stricker
Materials informatics – appreciation of data and algorithms
Materialwissenschaftliches Seminar TU Darmstadt, Germany

24.01.2024
F. Varnik
Shape memory polymers and their potential for energy storage applications
International Conference on Renewable Energies and Water Technologies ICREWT, Rabat, Morocco

29.01.2024
M. A. Stricker
Materials informatics – appreciation of data and algorithms
KCDS Talks – Computational and Data Science, Karlsruhe, Germany

14.02.2024
R. Drautz
Atomic cluster expansion fundamentals
Los Alamos National Laboratory, USA

14.02.2024
R. Drautz
Graph atomic cluster expansion: Accurate representation of atomic interactions for the simulation of materials properties
Los Alamos National Laboratory, USA

15.02.2024
M. A. Stricker
Mesoscale simulation of grain boundaries
MPIE Seminar, Düsseldorf, Germany

28.02.2024
R. Drautz
Atomic cluster expansion for simulating materials
Ruhr-Universität Bochum, Germany

18.03.2024
M. A. Stricker
Materials informatics – appreciation of data and algorithms
DPG Frühjahrstagung, TU Berlin, Germany

05.04.2024
S. Botti
Tuning electronic properties of hexagonal SiGe quantum wells
2nd International Workshop on Hexagonal SiGe and Related Materials, Milano, Italy

08.04.2024
R. Drautz
Atomic cluster expansion for modeling local and semilocal interactions
The Institute for Mathematical and Statistical Innovation, University of Chicago, USA

17.04.2024
A. Hartmaier
From discrete dislocation dynamics to a crystal plasticity/creep model for superalloys
Schöntal Symposium, Kloster Schöntal, Germany

14.05.2024
R. Drautz
Atomic cluster expansion and application to actinide chemistry and materials
Los Alamos National Laboratory, USA

15.05.2024
A. Hartmaier, R. Shoghi
Machine learning models for microstructure-property relationships
Tailor-made multiscale materials systems, 3rd International Workshop, Hamburg, Germany

16.05.2024
M. A. Stricker, A. Chauniyal, B. E. Udofia
Improving materials characterization by combining existing methods with machine learning
MRD Industry Day, ZGH, Bochum, Germany

21.05.2024
R. Drautz
Graph atomic cluster expansion and some applications
University of California, Berkeley, USA

12.06.2024
L. Zhang, M. A. Stricker
MatNexus: A comprehensive text mining and analysis suite for materials discovery
Science Slam for Materials Researchers, Ruhr- Universität Bochum, Germany

21.06.2024
R. Drautz
Atomic cluster expansion for a unified approach to machine learning potentials
CIMTEC 2024, Montecatini Terme, Italy

23.06.2024
R. Janisch, A. Azocar Guzman
Hydrogen trapping at grain boundaries and its effect on interfacial cohesion: The role of H chemical potential and residual stress
EPRI Hydrogen Embrittlement Workshop, University of Oxford, UK

24.06.2024
M. A. Stricker, B. E. Udofia, G. Lathiya, A. Chauniyal
Informatics for dislocations (and defects)
FAU Erlangen WW Seminar, Fürth, Germany

15.07.2024
M. A. Stricker
Materialinformatik – Wertschätzung von Daten und Algorithmen
KI4MAT Netzwerktreffen (ZENIT), Dillenburg, Germany

25.07.2024
R. Drautz
Efficient machine learning potentials
Computational Materials Science and Engineering GRC, Jordan Hotel at Sunday River, Newry, USA

25.07.2024
A. Grünebohm
Defects in ferroelectric oxides revisited
The 20th International Conference on Diffusion in Solids and Liquids DSL 2024, Barcelona, Spain

02.09.2024
R. Drautz
Machine learning potentials from the perspective of the atomic cluster expansion
Autumn School 2024 of CRC 1394, Aachen, Germany

04.09.2024
R. Drautz
A quick introduction to machine learning potentials and the atomic cluster expansion
SusMet School on Thermodynamics, Düsseldorf, Germany

10.09.2024
R. Drautz
Learning atomic interactions, summer school "Machine learning and materials discovery"
Institut Pascal, Paris-Saclay University, France

12.09.2024
R. Drautz
Learning atomic interactions
Mike Finnis 75th Birthday Symposium Imperial College, London, UK

12.09.2024
R. Janisch
1001 grain boundary stories
Mike Finnis 75th Birthday Symposium, Imperial College, London, UK

17.09.2024
R. Drautz
ACE with GRACE
GAP (M)ACE workshop, Berlin, Germany

23.09.2024
R. Janisch, A. Azocar Guzman
The role of chemical potential and residual stress on H trapping and embrittlement at grain boundaries: A first principles cohesive zone model
The 11th International Conference on Multiscale Materials Modeling, Prague, Czech Republic

23.09.2024
R. Drautz
Geometry, topology and atomic interactions – from fundamentals to accurate and efficient simulations
The 11th International Conference on Multiscale Materials Modeling, Prague, Czech Republic

10.10.2024
W. Peeters, V. van Lange, A. Belabbes, R. Farina, M. Vettori, S. Botti, J. Haverkort, M. van Tilburg, M. Jansen, M. van Hemert, M. Verheijen, F. Bechstedt
Hexagonal silicon germanium as a direct bandgap light source
PRiME 2024 Joint International Meeting, Honolulu, USA

14.10.2024
R. Drautz
Introduction to machine learning potentials for simulating surface segregation in alloys
SFB 1625 Colloquium, Bochum, Germany

19.11.2024
M. A. Stricker, S. Baghaee Ravari, M. Mahdavi Jafari, A. Chauniyal
Data-based approaches for interfaces
Characterization and Properties of Interface-Dominated Materials – InMa 2024 Symposium, Aachen, Germany

09.12.2024
R. Drautz
From electrons to materials design – the role of high-performance computing
Inauguration of RUB high-performance computing cluster Elysium, Bochum, Germany

► Contributed Talks and Posters

07.01.2023
A. Hartmaier, R. Shoghi, J. Schmidt, A. Biswas
Data-oriented constitutive modeling for plasticity and damage
International Conference on Plasticity, Damage, and Fracture 2023, Barcelo Bavaro Punta Cana, Dominican Republic

05.02.2023
A. Dimou
Thermal and elastic stability of dopants in $BaTiO_3$
Fundamental Physics of Ferroelectrics and Related materials 2023, Colorado School of Mines, Golden, USA

07.02.2023
A. Grünebohm, A. Dimou, R. Khachaturyan, S. Teng, P. Hirel
Multistep polarization switching on orthorhombic domain walls: A molecular dynamic study
Fundamental Physics of Ferroelectrics and Related materials 2023, Colorado School of Mines, Golden, USA

07.02.2023
R. Drautz
Atomic cluster expansion fundamentals
Workshop on development, validation and application of Atomic Cluster Expansion (ACE) models, Ruhr-Universität Bochum, Germany

20.03.2023
R. Shoghi, J. Schmidt, A. Hartmaier
Data-oriented constitutive models for polycrystalline metals
9th GAMM AG Data Workshop, Stuttgart, Germany

26.03.2023
R. Drautz
A very brief introduction to machine learning interatomic potentials
DPG-Frühjahrstagung 2023, Dresden, Germany

27.03.2023
S. Kunzmann
A systematic investigation of metastable phases in Niobium using density-functional theory
DPG-Frühjahrstagung 2023, Dresden, Germany

27.03.2023
T. K. Schmalofski, M. Kroll, R. Janisch, H. Dette
An efficiently automated method to sample the energies of grain boundaries
DPG-Frühjahrstagung 2023, Dresden, Germany

27.03.2023
S. Kunzmann, T. Hammerschmidt, G. Schierning, A. Grünebohm
Ab initio study of transition paths between (meta) stable phases of Nb and Ta-substitiuted Nb
DPG-Frühjahrstagung 2023, Dresden, Germany

27.03.2023
O. C. Sen, R. Janisch
Atomistic simulations of crack-tip interface interactions in lamellar TiAl microstructures
DPG-Frühjahrstagung 2023, Dresden, Germany

28.03.2023
R. Janisch, A. Neogi
Atomistic studies of crack tip twin-boundary interactions in lamellar TiAl alloys: Effect of misfit, misorientation and lamella spacing
DPG-Frühjahrstagung 2023, Dresden, Germany

28.03.2023
S. Teng, A. Dimou, A. Grünebohm
Impact of defect dipoles on ferroelectric domain-walls motion
DPG-Frühjahrstagung 2023, Dresden, Germany

30.03.2023
E. Ibrahim, Y. Lysogorskiy, R. Drautz
Atomic cluster expansion: Training a transferable water interatomic potential from the local atomic environments of ice
DPG-Frühjahrstagung 2023, Dresden, Germany

17.04.2023
L. Hsu, A. Grünebohm, F. Wendler
Field-direction-dependency of the electrocaloric effect
784. WE-Heraeus-Seminar, Physikzentrum Bad Honnef, Germany

21.05.2023
D. K. Nerella, M. A. Ali, H. F. Salama, V. Mohles, O. Shchyglo, I. Steinbach
Data-driven approach for estimating three-dimensional microstructural features of bainitic steels using phase-field simulation results
7th World Congress on Integrated Computational Materials Engineering (ICME 2023), Orlando, USA

23.05.2023
J. Schmidt, A. Hartmaier
Data-oriented description of microstructure-dependent plastic material behavior
7th World Congress on Integrated Computational Materials Engineering (ICME 2023), Orlando, USA

05.07.2023
R. Shoghi, A. Hartmaier
Developing a microstructure-sensitive machine learning yield function and strain hardening model
SEECCM Conference: 5th South-East European Conference on Computational Mechanics, Vrnjacka Banja, Serbia

05.09.2023
M. Burtscher, O. C. Sen, M. Alfreider, A. Chauniyal, R. Janisch, D. Kiener
Scale bridging evaluation of the fracture behavior of an advanced TiAl alloy
COMPLAS 2023, Barcelona, Spain

05.09.2023
T. K. Schmalofski, M. Kroll, P. Thome, H. Dette, R. Janisch
Active learning approach for grain boundary parameter space sampling
FEMS EUROMAT 2023, Frankfurt am Main, Germany

05.09.2023
R. Janisch, A. Neogi, O. C. Sen, A. Chauniyal
Deformation and fracture of lamellar γ-TiAl microstructures: Insights from atomistic simulations
FEMS EUROMAT 2023, Frankfurt am Main, Germany

06.09.2023
L. Zhang, M. A. Stricker
From text data to word embeddings in materials science
FEMS EUROMAT 2023, Frankfurt am Main, Germany

06.09.2023
M. A. Stricker, L. Banko, N. Sarazin, N. Siemer, J. Neugebauer, A. Ludwig
Computationally accelerated experimental materials characterization using pyiron
FEMS EUROMAT 2023, Frankfurt am Main, Germany

07.09.2023
B. E. Udofia, M. A. Stricker
Identification of dislocation structures in experimental Laue microdiffraction patterns
FEMS EUROMAT 2023, Frankfurt am Main, Germany

07.09.2023
L. Zhang, M. A. Stricker
Text mining for insights in material science: A case study in electrocatalysis
FEMS EUROMAT 2023, Frankfurt am Main, Germany

08.09.2023
M. A. Stricker
Materials informatics: Appreciation of data and algorithms
Project Meeting SPP1980, Duisburg, Germany

21.09.2023
D. K. Nerella, M. A. Ali, H. F. Salama, M. Tegeler, O. Shchyglo, I. Steinbach, M. Ackermann, J. Wang, O. Gülbay, S. Wesselmecking, U. Krupp, A. Durmaz, A. Thomas, T. Huschle, K. Karim, C. Eberl
iBain Automated intelligent-data-guided process design for fatigue-resistant steel components with bainitic microstructure
MaterialDigital general assembly, Karlsruhe Institute of Technology, Germany

05.10.2023
M. Uddagiri, P. G. Antala, O. Shchyglo, I. Steinbach
Dendrite operating state in directional solidification of AlCu binary system: Numerical benchmark test with OpenPhase software
Materials/Microstructure Modelling: Analytics & Benchmarks 2023, Karlsruhe, Germany

24.10.2023
L. Hsu
How can the electrocaloric effect be tuned by an electric field?
6th MRD ECR Day, Bochum, Germany

15.11.2023
L. Hsu
Field direction dependence of electrocaloric effect
The 9th Physics PhD Colloquium, Ruhr-Universität Bochum, Germany

01.12.2023
R. Shoghi, A. Hartmaier
A machine learning-based constitutive modeling of plastic behavior in polycrystalline materials using crystal plasticity simulations including strain hardening
MRS Fall Meeting & Exhibition, Boston, USA

18.03.2024
R. Janisch, A. Azocar Guzman
Effect of mechanical stress, chemical potential, and coverage on hydrogen solubility during decohesion of ferritic steel grain boundaries
DPG-Frühjahrstagung 2024, Berlin, Germany

18.03.2024
E. Ibrahim, Y. Lysogorskiy, R. Drautz
Transferable interatomic potential of water with the atomic cluster expansion
DPG-Frühjahrstagung 2024, Berlin, Germany

19.03.2024
L. Hsu
Epitaxial strain in arbitrary orientation in $BaTiO_3$ films and $BaTiO_3/SrTiO_3$ superlattices
DPG-Frühjahrstagung 2024, Berlin, Germany

19.03.2024
S. Kunzmann
Ab initio study of transition paths between (meta) stable phases of Nb and Ta-substituted Nb
DPG-Frühjahrstagung 2024, Berlin, Germany

19.03.2024
M. M. Namisi
Stability of mixed cation hybrid perovskites using DFT
DPG-Frühjahrstagung 2024, Berlin, Germany

22.03.2024
S. Teng
Towards precise domain-wall engineering in $BaTiO_3$-based materials
DPG-Frühjahrstagung 2024, Berlin, Germany

10.04.2024
Y. Schneider, A. Hartmaier
Advanced numerical methods in micromechanical finite element simulation of hydrogen diffusion with consideration of damage
Advanced Numerical Methods in Engineering Tasks, Technical University of Berlin, Germany

17.04.2024
M. A. Stricker
Materials informatics and data science
DAAD AINet, online

02.05.2024
A. Grünebohm
Defect dipoles in ferroelectrics – microscopic insights from ab initio based simulations
Fundamental Physics of Ferroelectrics, Washington DC, USA

02.05.2024
L. Hsu
Field direction dependence of ferroelectric transitions and electrocaloric effects
Fundamental Physics of Ferroelectrics, Washington DC, USA

09.05.2024
S. Teng
Phase coexistence and complex domain structures in $BaTiO_3$ induced by $SrTiO_3$ inclusions
XXV Jubilee Polish-Czech Seminar, Poznan, Poland

13.05.2024
L. Zhang, M. A. Stricker
A comparative study of machine learning models and vector analysis techniques for improved prediction of quaternary material systems based on word embeddings
Machine Learning Modalities for Materials Science (MLM4MS), Jožef Stefan Institute, Ljubljana, Slovenia

15.05.2024
B. E. Udofia
Identification of dislocation structures in experimental Laue microdiffraction patterns
Machine Learning Modalities for Materials Science (MLM4MS), Jožef Stefan Institute, Ljubljana, Slovenia

11.06.2024
L. Zhang, M. A. Stricker
MatNexus: A comprehensive text mining and analysis suite for materials discovery
7th Early Career Researchers Day, Ruhr-Universität Bochum, Germany

23.08.2024
M. A. Stricker, L. Banko, N. Sarazin, J. Janßen, N. Siemer, J. Neugebauer, A. Ludwig
Computationally accelerated experimental materials characterization using pyiron
Multiscale Materials Modeling 11, Prague, Czech Republic

27.08.2024
M. A. Stricker, L. Banko, N. Sarazin, J. Janßen, N. Siemer, J. Neugebauer, A. Ludwig
Computationally accelerated experimental materials characterization using pyiron
CRC1625 workshop: Designing the Future of Electrocatalysis with Compositionally Complex Solid Solutions, Bochum, Germany

19.09.2024
L. Zhang, M. A. Stricker
MatNexus: A tool for systematic text extraction and analysis in materials science
GC-MAC Summer School 2023, KIT Karlsruhe, Germany

23.09.2024
L. Zhang, M. A. Stricker
A comparative study of machine learning models and vector analysis techniques for improved prediction of quaternary material systems based on word embeddings
The 11th International Conference on Multiscale Materials Modeling, Prague, Czech Republic

24.09.2024
A. Hartmaier
Kanapy: An open software tool for analyzing and processing of microstructure data
MSE 2024 Materials Science and Engineerinig Congress and Exhibition, Darmstadt, Germany

25.09.2024
R. Shoghi, A. Hartmaier
A microstructure-sensitive machine learning model for plasticity and strain hardening in polycrystalline metals
MSE 2024 Materials Science and Engineerinig Congress and Exhibition, Darmstadt, Germany

25.09.2024
J. Schmidt, S. R. Kalidindi, A. Hartmaier
A texture-dependent yield criterion
MSE 2024 Materials Science and Engineerinig Congress and Exhibition, Darmstadt, Germany

25.09.2024
B. E. Udofia, M. A. Stricker
Identification of dislocation structures in experimental Laue microdiffraction patterns
The 11th International Conference on Multiscale Materials Modeling, Prague, Czech Republic

ICAMS

Seminars and other Lectures

14. Seminars and other Lectures

▶ Joint Seminar Series of ICAMS and the Institute for Materials

12.01.2023
Measuring individual layer mechanical behaviour of multilayers with X-ray diffraction
M. Cordill
Erich Schmid Institute for Materials Science, Leoben, Austria

31.10.2023
Shape programmable three-dimensional mesostructures and functional devices
Y. Huang
Northwestern University, Evanston, USA

16.11.2023
Understanding elementary deformation mechanisms in superalloys using advanced electron microscopy
M. J. Mills
The Ohio State University, Columbus, USA

18.01.2024
Data-driven interatomic potentials for inorganic materials chemistry
V. Deringer
University of Oxford, United Kingdom

06.06.2024
Grain growth and grain boundary migration in nano-crystalline materials under mechanical loads
C. Motz
Universität des Saarlandes, Saarbrücken, Germany

13.06.2024
Damage mechanisms in metals under complex loads – erosion, wear and multiaxial fatigue
S. Hanke
Universität Duisburg Essen, Duisburg, Germany

20.06.2024
A novel approach to parametrize a ferroelectric phase-field model from atomistic simulation data
F. Wendler
Friedrich-Alexander-Universität, Erlangen, Germany

04.07.2024
Deformation behaviour of P91 martensitic steel: Multiscale testing and crystal plasticity modelling
N. O'Dowd
University of Limerick, Ireland

07.11.2024
FE-FFT-based multiscale simulations of polycrystalline materials
J. Waimann
Ruhr-Universität Bochum, Germany

▶ Seminars and other Lectures

31.03.2023
Atomic cluster expansion with and without atoms
C. Ortner
University of Warwick, Coventry, United Kingdom

14.07.2023
Understanding the interplay of multiple mechanisms of hydrogen embrittlement using experiments and simulations
D. Mahajan
Indian Institute of Technology Ropar, India

14.11.2023
Study of the electronic, optical and photovoltaic properties of some types of halide-based semiconductors
O. L. El Hachemi
Hassan II University, Casablanca, Morocco

21.11.2023
Opto-electronic control domain manipulation in ferroelectric oxides
S. Pal
Queen Mary University of London, United Kingdom

18.01.2024
6th ICAMS Fireplace Conversation
M. Matsuo, M. Boeff
Otto Fuchs KG, Meinerzhagen and Siemens Energy, Mülheim a.d. Ruhr, Germany

25.01.2024
Feedbacks between stress and chemical processes in rocks and other crystalline materials
J. Wheeler
University of Liverpool, United Kingdom

14.02.2024
Insight into CO_2 capture in biphasic solvents: molecular dynamics simulations using reactive force fields and experimental verification
M. Kanani
Shiraz University, Iran

03.04.2024
Models for diffusion creep with implications for metallurgy and geology
J. Wheeler
University of Liverpool, United Kingdom

03.04.2024
Investigation of dislocation structure evolution using dark-field X-ray microscopy
F. T. Frankus
Technical University of Denmark, Kongens Lyngby, Denmark

10.06.2024
Stochastic theory of ferroelectric domain structure formation dominated by quenched disorder
O. Mazur
Technical University of Liberec, Czech Republic

12.09.2024
7th ICAMS Fireplace Conversation
A. Harjunmaa
Accenture Song Content, Stuttgart, Germany

11.11.2024
Ultrafast control of quantum materials using intense laser fields
N. Tancogne-Dejean
Max Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany

27.11.2024
Machine-learning assisted design of solid-state batteries
F. Marsusi
Ruhr-Universität Bochum, Germany

27.11.2024
Lithium-based electrides superconductors under high pressure
W. Cui
Jiangsu Normal University, Xuzhou, China

ICAMS

Teaching

15. Teaching

► MSS (Master) lecture courses summer term 2023

J. Kundin
The CALPHAD method

A. Hartmaier
Computational plasticity

R. Drautz
Data-driven materials science

T. Hammerschmidt, R. Janisch
Interfaces and surfaces

G. Sutmann
Introduction to parallel- & scientific computing

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 (Master) lecture courses winter term 2023/24

A. Grünebohm, M. Mrovec
Advanced atomistic simulation methods

Y. Lysogorskiy
Advanced statistical methods in materials science

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

R. Drautz
Atomistic simulation methods

A. Hartmaier
Computational fracture mechanics

I. Steinbach
Continuum methods in materials science

A. Grünebohm, M. Piacenza, M. Stricker
Documenting and communicating science

G. Eggeler
Elements of microstructure

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

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

M. Stricker
Materials informatics

R. Janisch
Multiscale mechanics of materials

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

A. Hartmaier, F. Varnik
Statistical mechanics and fundamental materials physics

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

► MaWi (Bachelor) lecture courses winter term 2023/24

R. Drautz
Material- und Festkörperphysik 1

T. Hammerschmidt
Programmierung und numerische Methoden

► Block course on modelling – University of Oxford, 12.11.2023 – 17.11.2023

R. Drautz (jointly with Professor Jonathan Yates)
Introduction to modelling in materials science

► MSS (Master) lecture courses summer term 2024

J. Kundin
The CALPHAD method

A. Hartmaier
Computational plasticity

R. Drautz
Data-driven materials science

T. Hammerschmidt, R. Janisch
Interfaces and surfaces

G. Sutmann
Introduction to parallel- and scientific computing

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

► MaWi (Bachelor) lecture courses summer term 2024

M. Stricker
Computational materials science 1: Anwendungen und Software

M. Stricker
Fortgeschrittene Programmiermethoden

A. Grünebohm
Material- und Festkörperphysik 2

► MSS (Master) lecture courses winter term 2024/25

A. Grünebohm, M. Mrovec
Advanced atomistic simulation methods

Y. Lysogorskiy
Advanced statistical methods in materials science

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

R. Drautz
Atomistic simulation methods

A. Hartmaier
Computational fracture mechanics

I. Steinbach
Continuum methods in materials science

A. Grünebohm, M. Piacenza, M. Stricker
Documenting and communicating science

T. Li
Elements of microstructure

A. Hartmaier
Fundamental materials physics

T. Hammerschmidt, M. Mrovec
Interatomic potentials

T. Li
Introduction to 3-dimensional materials characterization techniques

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

A. Hartmaier et al.
Materials modelling lab

R. Janisch
Multiscale mechanics of materials

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

F. Varnik
Thermodynamics and statistical mechanics

► **MaWi (Bachelor) lecture courses winter term 2024/25**

A. Hartmaier
Computational Materials Science 2: Einführung in die Kontinuumsmethoden

F. Varnik
Einführung in die CALPHAD-Methode

T. Hammerschmidt
Materialinformatik

J. Kundin
Modellierung von Diffusionsprozessen in Werkstoffen

R. Janisch
Oberflächen und Grenzflächen: Modelle, Prozesse, Eigenschaften

► **Block course on modelling – University of Oxford, 17.11.2024 – 22.11.2024**

R. Drautz (jointly with Professor Jonathan Yates)
Introduction to modelling in materials science

► **ICAMS Graduate School**

A. Grünebohm, M. Stricker
PhD seminar: 17.03.2023

Part I: Atomistic modelling and simulation, block course from 21.–22.09.2023

PhD seminar: 06.10.2023

PhD seminar: 05.04.2024 (cancelled)

Part II: Micromechanical modelling, block course from 30.09.–01.10.2024

PhD seminar: 11.10.2024

► **Rutopia Panel Discussions**

A. Grünebohm, T. Li
Rutopia – What is a PhD about? - 26.04.2023

Rutopia – Is ChatGPT good for my research? – 03.07.2024

Rutopia – Share your stories: Survive the German academic system with diverse backgrounds - 14.11.2024

► **Solarup Summer School at ICAMS**

S. Botti
PhD seminar: 09.–11. 09. 2024 (EU project)

► **EUSpeclab Summer School at ICAMS**

M. Marques
PhD seminar: 16.– 20. 09. 2024 (EU project)

ICAMS

ICAMS Members 2023 and 2024

16. ICAMS Members 2023 and 2024

▸ Staff at ICAMS 2023 and 2024

About 50 –70 researchers, including PhD students, work at ICAMS; about 6 administrative staff and 4 technicians support the institute.

Figure 19.1 shows the development of ICAMS staff numbers through the past fourteen 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. 2017 to 2020 the number of employees has leveled off at around 80. There has been a slight decline in the number of employees since 2020, but a number of new hires are planned from spring 2025 due to several new projects.

ICAMS' research staff is very international. This is one of the reasons why our staff numbers have been affected by the pandemic in the past years. The majority of ICAMS scientists hold a degree in engineering and materials science, followed by degrees in physics, chemistry and mathematics or computer science (*Fig. 19.2*). This educational diversity of our research staff provides the basis for ICAMS' interdisciplinary research.

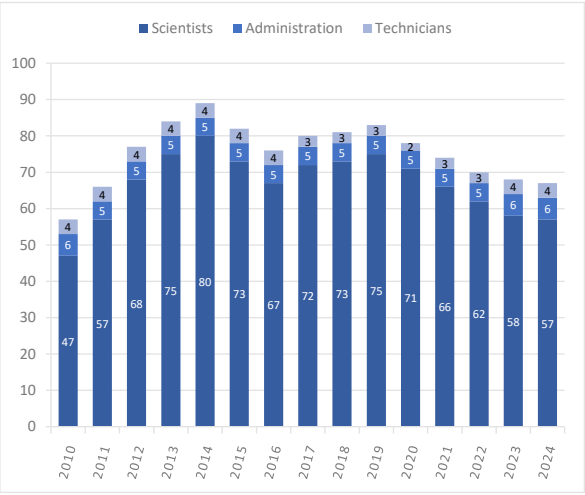


Fig. 19.1: Development of ICAMS staff from 2010 to 2024.

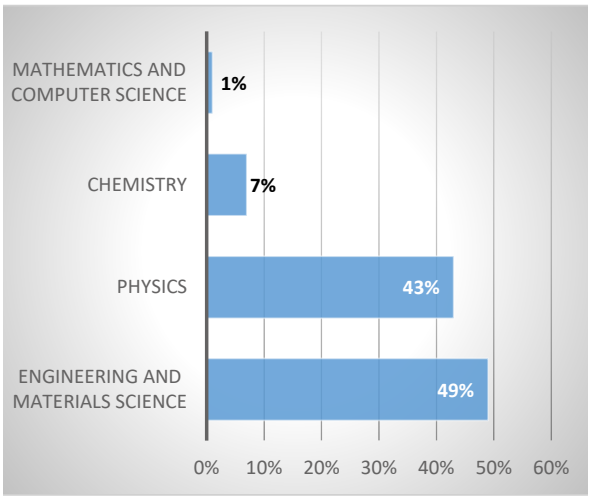
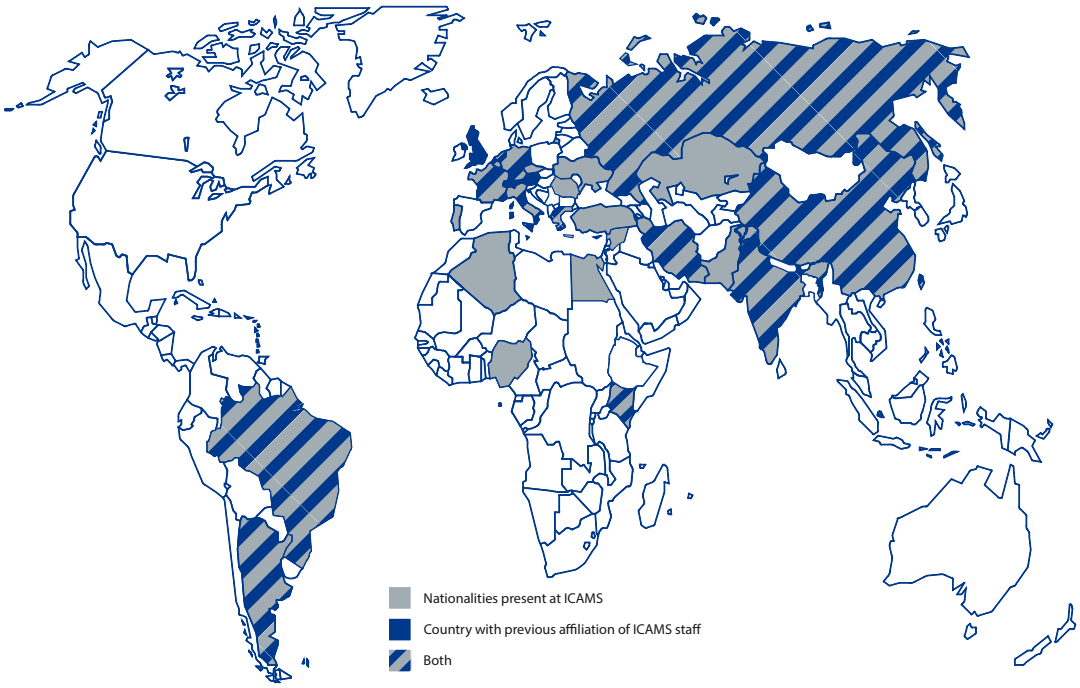


Fig. 19.2: Breakdown of first degree of ICAMS researchers in 2023/2024.

In 2023 and 2024 researchers from 25 different countries were working at ICAMS (see grey areas in *Fig.19.3*). 21% of the ICAMS staff is of German and 79% of foreign nationality. For ICAMS, it is of vital importance to attract talented scientists from leading research institutions worldwide.

Figure 19.3 gives an overview of the countries and institutions of origin of the current ICAMS researchers. 13 of the 47 institutions are located in Germany, 17 in other EU countries and 17 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 Martín

Austria
Technical University of Vienna

Belgium
UC Louvain

Brazil
Instituto Militar de Engenharia

China
Beihang University, Peking
Central South University, Changsha
Chongqing Univ. of Science and Tech.
Jiangsu National University
Nanchang Hongkong University

France
CEA Grenoble
LEM-ONERA-CNRS, Chatillion
Nantes Université
Université de Paris Cité

Germany
AICE, Aachen
Fraunhofer IWM, Freiburg
Friedrich-Alexander Univ., Erlangen-Nürnberg
Friedrich-Schiller Universität Jena
Otto von Guericke Universität Magdeburg
Martin-Luther Universität Halle-Wittenberg
Ruhr-Universität Bochum
RWTH Aachen
TU Chemnitz
TU Dortmund
TU Dresden
Universität Bayreuth
Universität Duisburg-Essen

Greece
University of Ioannina

India
Central University of Haryana
Centre for Excellence in Basic Sciences (CEBS), Nalanda
Indian Institute of Technology, Delhi
Indian Institute of Technology, Hyderabad
Indian Institute of Technology and Science (BITS), Pilani

Iran
Sharif University of Technology, Teheran
Shiraz University
University of Teheran

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

Kenya
University of Nairobi

Russia
Kazan Federal University
JIHT Moskow

Switzerland
EPFL, Lausanne

Taiwan
National Chiao Tung University

The Netherlands
TU Delft

United Kingdom
Imperial College London
University of Oxford

Fig. 19.3: 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. Muhammad Adil Ali
Postdoctoral Researcher
Scale-Bridging Thermodynamic and Kinetic Simulation

Dr. Ayoub Aouina
Postdoctoral Researcher
Computational Design of Functional Interfaces

M.Sc. Sepideh Baghaee Ravari
Doctoral Candidate
Materials Informatics and Data Science

Dr. Preeti Bhumla
Postdoctoral Researcher
Computational Design of Functional Interfaces

Lukas Blacha
IT System Administration
IT

Dr. Anton Bochkarev
Postdoctoral Researcher
Atomistic Modelling and Simulation

Prof. Dr. Silvana Botti
Head of Department
Computational Design of Functional Interfaces

Dr.-Ing. Pierre-Paul De Breuck
Postdoctoral Researcher
Artificial Intelligence for Integrated Material Science

Dr.-Ing. Théo Cavignac
Postdoctoral Researcher
Artificial Intelligence for Integrated Material Science

Dr.-Ing. Ashish Chauniyal
Postdoctoral Researcher
Materials Informatics and Data Science
(at ICAMS until 31.03.2024)

M.Sc. Xiao Chen
Doctoral Candidate
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Dipl.-Eng. Aris Dimou
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Scale-Bridging Simulation of Functional Composites
(at ICAMS until 14.11.2023)

Prof. Dr. Ralf Drautz
Head of Department
Atomistic Modelling and Simulation

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(at ICAMS until 31.12.2023)

Dr. Mariano Daniel Forti
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Prof. Dr. Anna Grünebohm
Head of Department
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Christa Hermichen
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M.Eng. Daysianne Kessy Mendes Isidorio
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Dr. Hossein Jafarzadeh
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(at ICAMS until 14. 07. 2023)

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Dr. Tushar Jogi
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Dipl.-Des., M.A. Jutta Kellermann
MSS Examination Office Administration
Coordination Office

Patrick Klein
IT System Administration
IT

Deborah Kowolik
Personal Assistant
Artificial Intelligence for Integrated Material Science

M.Sc. Rohan Kumar
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Dr. habil. Julia Kundin
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M.Sc. Susanne Kunzmann
Doctoral Candidate
Scale-Bridging Simulation of Functional Composites

Alina Larraß
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Dr. Yury Lysogorskiy
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Prof. Dr. Miguel A. L. Marques
Head of Department
Artificial Intelligence for Integrated Material Science

Eva Masuch
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Dipl.-Inform. Lothar Merl
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IT

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Materials Informatics and Data Science

PD Dr. habil. Volker Mohles
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(at ICAMS until 30. 09. 2024)

M.Sc. Sumit Mondal
Doctoral Candidate
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(at ICAMS until 31.08. 2024)

Dr. Matous Mrovec
Research Group Leader
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M.Sc. Reza Namdar
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation

M.Sc. Mauwa Mwanaidi Namisi
Doctoral Candidate
Scale-Bridging Simulation of Functional Composites

M.Sc. Dhanunjaya Kumar Nerella
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation

M.Sc. Feng Pan
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Micromechanical and Macroscopic Modelling

Dr. Anastasiia Petrova
Postdoctoral Researcher
Atomistic Modelling and Simulation

Dr. Manuel Piacenza
Head of Coordination Office
Coordination Office

Dr. Isabel Pietka
Doctoral Candidate
Atomistic Modelling and Simulation
(at ICAMS until 31.12.2023)

M.Sc. Minaam Qamar
Doctoral Candidate
Atomistic Modelling and Simulation

Dr. Lin Qin
Postdoctoral Researcher
Atomistic Modelling and Simulation
(at ICAMS until 30.04.2023)

M.Sc. Senja Josepha Johanna Ramakers
Doctoral Candidate
Atomistic Modelling and Simulation
(at ICAMS until 31.03.2023)

Dr. Matteo Rinaldi
Postdoctoral Researcher
Atomistic Modelling and Simulation
(at ICAMS until 31.10.2023)

Dr. Ahmadreza Riyahi Khorasgani
Postdoctoral Researcher
Scale-Bridging Thermodynamic and Kinetic Simulation

Dr.-Ing. Hafiz Muhammad Sajjad
Postdoctoral Researcher
Micromechanical and Macroscopic Modelling
(at ICAMS until 31.12.2024)

M.Sc. Hesham Fathy Mohamed Ali Salama
Doctoral Candidate
Scale-Bridging Thermodynamic and Kinetic Simulation

Dr. Raphael Schiedung
Postdoctoral Researcher
Scale-Bridging Thermodynamic and Kinetic Simulation

Dr. Timo Klaus Schmalofski
Doctoral Candidate
Micromechanical and Macroscopic Modelling
(at ICAMS until 14.11.2023)

M.Sc. Jan Schmidt
Doctoral Candidate
Micromechanical and Macroscopic Modelling

Dr.-Ing. Yanling Schneider
Postdoctoral Researcher
Micromechanical and Macroscopic Modelling
(at ICAMS until 31.12.2024)

M.Sc. Onur Can Sen
Doctoral Candidate
Micromechanical and Macroscopic Modelling

M.Sc. Preeti Sharma
Doctoral Candidate
Computational Design of Functional Interfaces

Dr. Oleg Shchyglo
Research Group Leader
Scale-Bridging Thermodynamic and Kinetic Simulation

M.Sc. Ronak Shoghi
Doctoral Candidate
Micromechanical and Macroscopic Modelling

M.Sc. Sidrah Sidrah
Doctoral Candidate
Micromechanical and Macroscopic Modelling

Dr. Sergei Starikov
Postdoctoral Researcher
Atomistic Modelling and Simulation

Prof. Dr. Ingo Steinbach
Head of Department
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