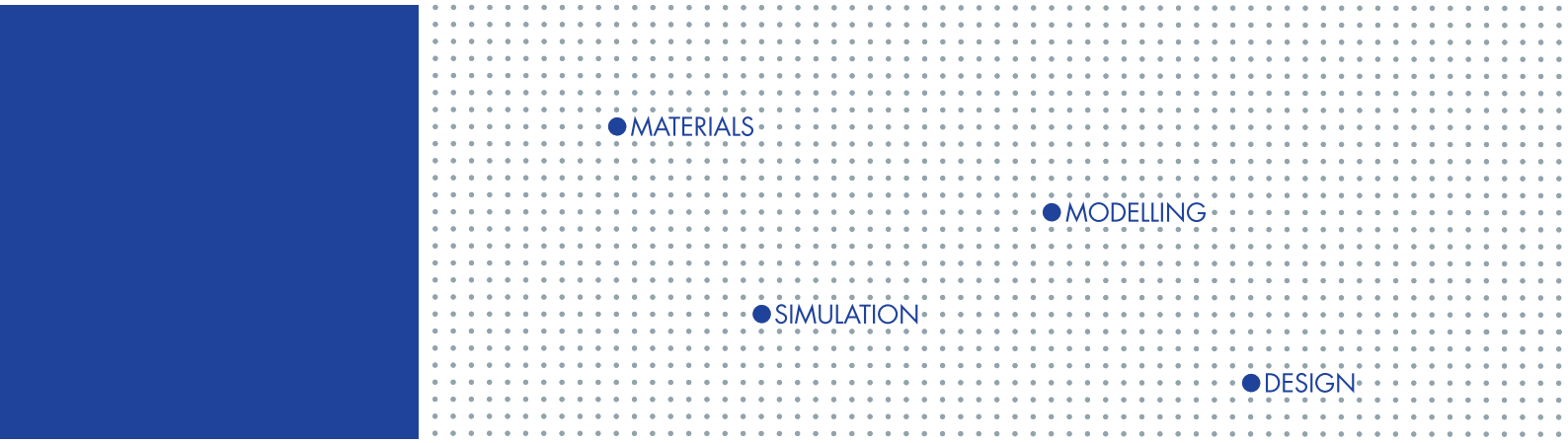
Scientific Report 2021 and 2022



ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS

Scientific Report 2021 and 2022

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Germany

Preface

The simulation of material properties at all length- and timescales is our institute's primary challenge. Over the years ICAMS has grown and extended its activities to new methods and new classes of materials. Software development and application of data science and machine-learning based methods go hand in hand with applications in various fields. This report summarizes our research and teaching activities in the past two years. New professors have been appointed and new study programs have been launched and new research programs have been started. The first workshops and conferences after the pandemic are taking place in person again.

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 success.

We hope you enjoy reading.

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Managing Director

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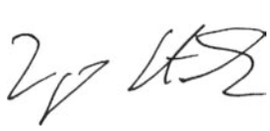
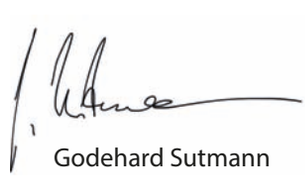
Alexander Hartmaier

Markus Stricker



Ingo Steinbach



Godehard Sutmann

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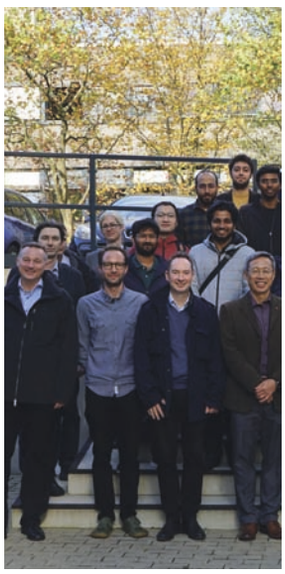

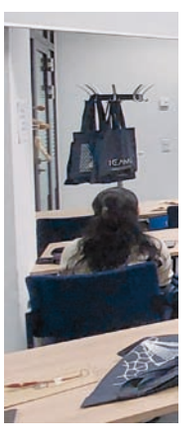




▸ ICAMS in 2021 and 2022

ICAMS is the interdisciplinary centre for advanced materials simulation. The research of ICAMS covers all length and time scales of relevance for properties of materials: electronic, atomic, micro and macro. Simulations carried out at ICAMS target the discovery and design of new materials. ICAMS develops theories and models, and methods and software for the simulation of materials and to this end combines first-principles theories with high-throughput computation, data science and machine learning. ICAMS educates the next generation of materials scientists by providing research-driven teaching that covers the breadth of modern multidisciplinary materials theory and experimentation.

In 2021 and 2022 ICAMS actively developed and expanded its research and teaching portfolio, including the following:

- A new full professorship 'Artificial intelligence for integrated materials design' was established,
- A new Bachelor program 'Materialwissenschaft' (materials science) was launched,
- ICAMS made leading contributions to the proposal for the next round of the Excellence Strategy and to several other collaborated projects.

New Professorship 'Artificial intelligence for integrated materials design'

Professor Miguel Marques from Universität Halle has been appointed to the position of a full professor in 'Artificial intelligence for integrated materials design'. Professor Marques will be fully integrated into ICAMS, while also being part of the Research Center Future Energy Materials Systems. The group of Professor Marques will be housed in the ZGH research building.

Professor Marques is a leader for the computational discovery of novel materials. His research interests focus on density functional theory, super conductivity and machine learning in materials science.

Simultaneously with Professor Marques, Professor Silvana Botti has been appointed as a full professor in the Department of Physics and Astronomy, also within the context of the Research Center Future Energy Materials Systems. As Professor Marques, Professor Botti is a leader in the computational development of novel materials, with a focus on the computation of excited states in solids. Professor Botti will also be closely associated to ICAMS.

Fig. 2.1: Prof. Dr. Miguel Marques and Prof. Dr. Silvana Botti (Photos Katja Marquard, RUB).

▸ Excellence Strategy and collaborative projects

As part of its mission, ICAMS supports collaborative research projects with modelling and simulation. Five of 25 PIs of the next materials science proposal for the excellence initiative will be associated to ICAMS and take responsibility for theory and simulation, while ICAMS is also part of the small core team that currently drives the proposal. ICAMS will further be part of the upcoming proposal of excellence cluster RESOLV. Together with groups from other faculties, ICAMS takes a leading role in the cross-departmental research areas atomistic simulations and data driven materials research and thus contributes to RUB's outstanding strength in these fields.

ICAMS is part of several other collaborative projects, most notably the CRC TR 103 'From atoms to turbines blades' headed by Gunther Eggeler, where ICAMS contributes five partial projects. In the past two years ICAMS has supported several proposals for continuation and the establishment of new CRCs, all of which will be reviewed in 2023 and 2024

▸ Teaching

Bachelor program in Materials Science

The new Bachelor course "Materialwissenschaft" started in the winter term 2021/22. The curriculum was developed by ICAMS and the Institute for Materials, the faculty of Mechanical Engineering hosts the course. The course language is German. The first students have successfully started the program.

Master's course Materials Science and Simulation (MSS)

In 2021 we received more than 1200, and in 2022, almost 1600 applications for our master's programme "Materials Science and Simulation". Altogether 44 students eventually took up their studies in the last two years. 20 master's students successfully graduated in 2021 and 12 in 2022.

Due to the pandemic situation, no excursions could be offered to MSS students in 2021 and 2022. The next excursion will take place at the end of May 2023. Companies in Berlin and Wolfsburg are to be visited.

In January 2022, a fireplace talk on the topic "Foundation as a third career path at the university" was offered as an online event in collaboration with the the Worldfactory Start-up Center of the RUB and the Incubator Materials.

The MSS Master Fair 2021 took place as an online event but in the winter semester 2022/23 we were able to return to a face-to-face event. The ICAMS professors gave an overview about the research fields of their departments and presented master's thesis topics.

Graduate School

ICAMS has established a graduate school for scale-bridging materials modelling at Ruhr-Universität Bochum. Its target group are doctoral candidates with their research focus on materials modelling, either from ICAMS, the ICAMS Advanced Study Groups or the Materials Research Department. The goal of the programme is the education of our students. In 2021 and 2022 block courses on "The phase-field approach" and "Micromechanical and macroscopic modelling" took place, furthermore four PhD seminars were held.

Max Planck Research School SusMet

The Max Planck Research School on Sustainable Metallurgy started in 2022. It offers 38 PhD positions and is coordinated at the MPIE in Düsseldorf. ICAMS is one of the project partners.

Fig. 2.2: MSS fresher's day 2022. Top: Welcome and introduction to the ICAMS CIPpool. Bottom left: Seniors took the freshers to the RUB Botanical Garden.

Fig. 2.3: The ICAMS Masterfair took place in presence in the winter semester 2022/23.

▸ Workshops and Conferences

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

At the 2021 Potentials: Workflows for atomistic simulation leading international researchers gave an introduction to simulations and workflows that they use in their research. In the afternoons hands-on tutorials using pyiron enabled the participants to set up their own simulation tasks and workflows.

At the 2021 Advanced Discussions: Recent trends in material design, participants from academia and industry presented and discussed recent developments in the fields of data-driven methods in material design, metals and microstructures, and functional materials.

The 2021 Materials Chain International Conference was dedicated to Materials Discovery and Processing for Energy. International speakers from various disciplines presented results in the areas materials for

physical energy conversion, 2D and hybrid functional materials, magnetic materials for energy conversion, metals and alloys, and production engineering and additive manufacturing.

The 2022 edition of the ICAMS Advanced Discussions featured the current state and future direction of the modeling of microstructure evolution in structural and functional materials. A special focus was laid on the extraction of process-microstructure-property relationships based on microstructural and scale-bridging simulation.

The three-day workshop "Potentials from electrons to phase diagrams" provided tutorials and hands-on classes covering the complete chain from high-throughput electronic structure calculations to the computation of phase diagrams.

Materials with complex phase transitions and/or complex composition may be the key to improve caloric materials. Local, national and international experts presented and discussed their research on fundamental aspects of functional phase transitions and new routes for their optimization during the workshop Phases: Complex Phase Transitions with Functional Properties.

The 2022 Materials Chain International Conference was focused on Future Energy Materials and Systems. The covered areas of interest were machine learning and ai methods, electrocatalysis, energy storage, and coatings and processing.

Furthermore, ICAMS scientists were members of the scientific panels or contributed to the organisation of conferences and workshops, including symposia and sessions at several international conferences:

2021

- Platform for Advanced Scientific Computing, PASC conference
- CECAM Workshop Virtual Materials Design
- CECAM Flagship Workshop Advances in Electrostatic Calculations: the road towards Exascale
- Online Workshop Materials Data Science for Accelerating Materials Discovery and Design
- DGM Working Group Microstructural Mechanics, Freiburg i.Br.

2022

- Data-Driven Materials Science at DPG Spring Meeting, Regensburg
- Platform for Advanced Scientific Computing, PASC conference, Basel
- EuroSuperalloys, Bamberg
- MSE Congress, Darmstadt
- DGM Working Group Microstructural Mechanics, Bochum

Fig. 2.4: ICAMS Advanced Discussions 2022.

Fig. 2.5: SFC-workshop "Complex Phase Transitions with Functional Properties" at the RUB.

Fig. 2.6: AMS-workshop "Potentials" at Schloss Reisensburg.

▸ Equal Opportunity Projects

In June 2021, ICAMS, the Materials Research Department, and the SFB/TRR 103 organized the online film screening and discussion event "Picture a Scienctist". It was supported by the RUB Institute for Gender Studies, the project "Unser Campus", and RUB's Department for Organisational and Professional Development. Experts from the above mentioned institutions provided additional information about gender equality policy at RUB and related topics.

The new "Summer School Materialwissenschaft" is intended to give students (f/d) 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. Start is in summer 2023.

Fig. 2.7: Advertisement for the online screening and discussion "Picture a Scientist".

▸ Outing

The first ICAMS outing after the pandemic took the participants to Haltern. A hike through the Westruper Heide and a visit to a climbing park and an archery range were on the agenda. The long-missed social interaction was gratefully accepted!

Fig. 2.8: Outing to Haltern 2022.

ICAMS

Organisation of ICAMS

3. Organisation of ICAMS

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Prof. Dr. Markus Anthony Stricker

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

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Coordination O ce

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MSS-Examination O ce

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ICAMS

Department Atomistic Modelling and Simulation AMS

4. Department Atomistic Modelling and Simulation

Prof. Dr. Ralf Drautz

▸ Research

Within the materials modelling activities of the three ICAMS departments, the department of Atomistic Modelling and Simulation works on the finest, most fundamental length scale of atomistic simulations.

Our research has three main objectives:

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

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

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

Atomistic simulations focus on predicting structural and mechanical properties of materials and phase diagrams. In this way a coherent link from the electronic structure to the continuum description of materials on the meso- and macroscale is obtained.

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

Density functional theory calculations and machine learning are employed for computational materials design and assist and guide experimental research.

▸ Structure

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

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

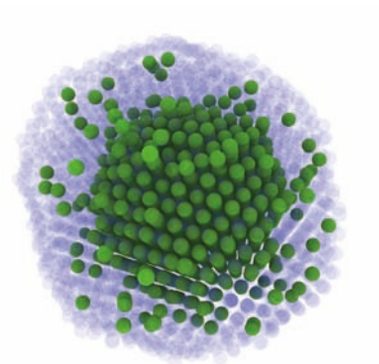


Fig. 4.1: Simulation of intermixing in a Pt-Rh cluster at high temperature. Rh atoms in green, Pt atoms in transparent blue.

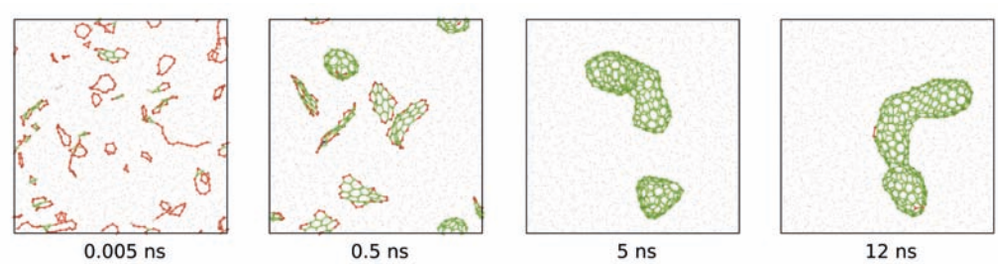


Fig. 4.2: Simulation of carbon fullerene formation in an argon atmosphere at high temperature. Carbon atoms in green, argon atoms are only faintly visible.

AMS

4. 1. Atomistic Simulation of Structural and Phase Stability

Group leader:
PD Dr. habil. Thomas Hammerschmidt

Group members:
Dr. Mariano Forti
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), the complexity of the microstructures (e.g. dislocations and precipitates in steels) and the complexity of the physical phenomena (e.g. magnetic phase transition in iron, finite-T properties of battery materials, dislocations in high-entropy alloys).

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

▸ Competences

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

Tight-binding bond parameters for dimers across the periodic table from density-functional theory

In this work, we parametrize TB bond parameters for nearly all combinations of elements of period 1 to 6 and group 3 to 18 of the periodic table. By downfolding the dimer DFT wave function in the Harris-Foulkes approximation to a minimal basis, we obtain the non-orthogonal TB Hamiltonian matrix, the overlap matrix and the Löwdin-orthogonalized TB Hamiltonian matrix for 1711 homo-atomic and hetero-atomic dimers. The TB eigenvalues compare well to their DFT reference over a wide range of interatomic distances. The TB matrix elements are smooth functions that are parameterized efficiently with only few exponential functions. We demonstrate that the TB matrix elements follow intuitive chemical trends across the elements. By comparing to well-known qualitative TB models, we rationalize and point out the limitations of the rectangular d-band model, a reduced TB model for sp systems and canonical TB models for sp-valent and d-valent systems. We briefly compare our parametrizations to NRL-TB and DFTB; a more detailed comparison requires taking into account the screening of the dimer bond integrals when they are immersed in the bulk. The parameters for the 1711 dimers serve as starting point for the parametrization of TB/BOP models.

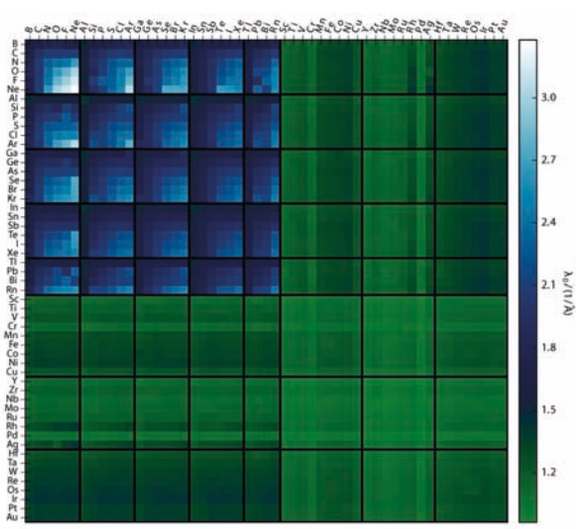


Fig. 4.3: Parameters (inverse decay length) of orthogonal tight-binding models of homoatomic and heteroatomic dimers across the periodic table obtained from downfolding the DFT eigenspectrum to a tight-binding minimal basis.

J. Jenke, A. N. C. Ladines, T. Hammerschmidt,
D. G. Pettifor, R. Drautz,
Tight-binding bond parameters for dimers across the periodic table from density-functional theory,
PhysRevMaterials, 5, 023801, 2021

Influence of spin fluctuations on structural phase transitions of iron

Iron changes its crystal structure from α (bcc) to γ (fcc) to δ (bcc) with increasing temperature. We apply a magnetic, orthogonal, d-valent TB model to clarify the influence of spin fluctuations on these structural phase transitions. The interplay between spin fluctuations and atomic vibrations is included by computing the effect of spin fluctuations on phonons, using a spin-space averaging scheme and spin-space sampling by Hamiltonian Monte Carlo. The magnetic/electronic contribution to the free energy is determined by thermodynamic integration along the Bain path between bcc and fcc. In this way, we are able to compute the temperature-dependent vibrational and magnetic/electronic contributions to the phase transitions of iron within a consistent framework at the TB level. Our computed temperature-dependent vibrational and magnetic/electronic contributions to the free energy of bcc and fcc iron show that spin fluctuations influence the α - γ and the γ - δ phase transitions via different mechanisms. The first mechanism, the influence of spin fluctuations on the magnetic-free energy, decreases the free energy of bcc iron relative to that of fcc iron with increasing temperatures and impacts the α - γ phase transition. The second mechanism, the spin-lattice coupling, increases the free energy of bcc iron relative to that of fcc iron and impacts the γ - δ phase transition. By adding the vibrational and the magnetic/electronic contribution to the free-energy difference, we can reproduce the experimentally observed sequence of structural phase transitions with phase-transition temperatures of around 1050 K and 1600 K in good agreement with experiment. Our framework with a magnetic TB Hamiltonian can hence explain the microscopic origin of the structural phase transitions in iron.

N. Wang, T. Hammerschmidt, T. Hickel, J. Rogal, R. Drautz,
Influence of spin fluctuations on structural phase transitions of iron,
Phys Rev B, accepted

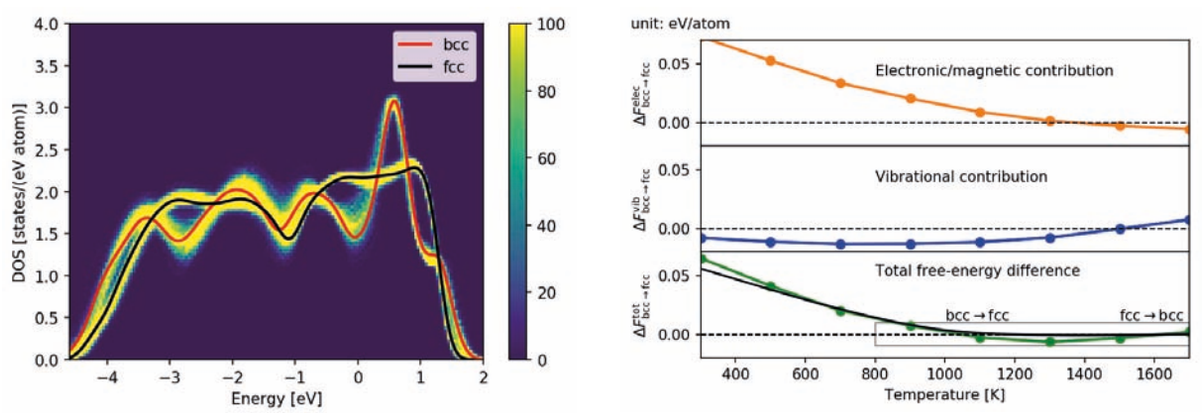


Fig. 4.4: (Left) Histograms of electronic density of states of bcc and fcc iron at 1500K sampled for 1000 magnetic configurations. (Right) Electronic (orange), vibrational (blue) and total free-energy differences (green) between bcc and fcc iron versus temperature computed with TB and with CALPHAD (black).

Magnetic bond-order potential for iron-cobalt alloys

We developed an analytic bond-order potential for Fe-Co alloys. We use a d-valent orthogonal tight-binding Hamiltonian in two-center approximation and employ an embedding function to account for the s electrons. The functional form is physically transparent and requires only a small set of reference data for parameterization. The underlying physical model ensures robust predictions for properties of Fe-Co that we did not include in the fit. We demonstrate the transferability of our potential to various material properties: phase stability of ordered and disordered alloys, elastic constants and phonons, point defects, structural transformations, and planar defects. Due to the explicit treatment of magnetism, our BOP reproduces the main features of the DFT electronic structure for magnetic and nonmagnetic phases. Further, the BOP reproduces the dense sequence of ground-states of Fe-rich Fe-Co alloys with an accuracy of about 10 meV to previous DFT results as well as the stabilization of B2 against disordered phases by magnetism. The analytic BOP for magnetic Fe-Co paves the way to atomistic simulations of Fe-Co alloys with a reliable treatment of magnetism at length and time scales not accessible with DFT.

A. Egorov, A. Subramanyam, Z. Yuan, R. Drautz, T. Hammerschmidt,
Magnetic bond-order potential for iron-cobalt alloys, Phys Rev Materials, under review

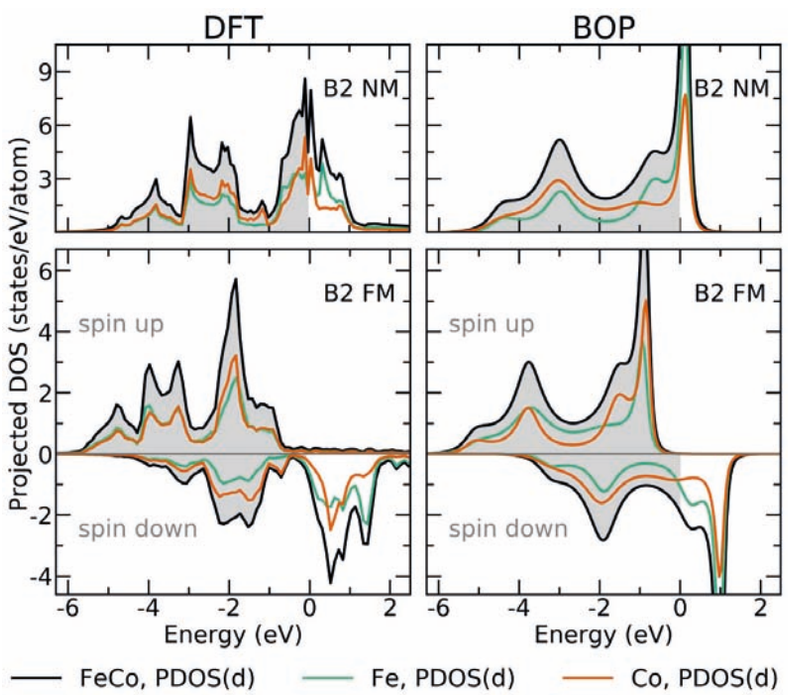


Fig. 4.5: Electronic DOS of d-orbitals of B2 FeCo with non-magnetic (NM) and ferromagnetic (FM) configurations obtained with DFT (left) and BOP (right). The Fermi energy is taken as 0 eV.

AMS

4.2. Atomistic Simulation of Mechanical Behaviour

Group leader:
Dr. Matous Mrovec

Group members:
Minaam Qamar
Dr. Sergei Starikov

▸ Research

The primary goal of the research group is to understand phenomena that occur on the atomic scale and that are related to macroscopic mechanical behaviour. We start with modelling 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 interatomic potentials. Recently, we have focused on the development and application of atomic cluster expansion (ACE) models that can reach the accuracy and transferability of electronic structure methods while remaining highly computationally efficient and applicable in large-scale atomistic simulations. We also integrate atomistic simulations and mesoscale techniques (DDD, kMC), phenomenological and continuum theories as well as experiments.

▸ Competences

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

Atomic cluster expansion for quantum-accurate large-scale simulations of carbon

We have recently developed an atomic cluster expansion (ACE) for carbon, which presents a significant improvement over available classical and machine learning potentials. The ACE was parameterized based on an exhaustive set of important carbon structures that were computed using accurate density functional theory (DFT) calculations. Our extensive validation tests revealed that ACE is able to predict a broad range of properties of molecular, liquid, crystalline, and amorphous carbon phases while being several orders of magnitude more computationally efficient than available machine learning models.

The outstanding predictive power of ACE was demonstrated on three distinct applications: a brittle crack propagation in diamond, an evolution of amorphous carbon structures at different densities and quench rates, and nucleation and growth of fullerene clusters under high pressure and temperature conditions.

The key ingredient of constructing any ACE model is an accurate and consistent reference dataset that covers a large part of the phase space of atomic configurations. Such a dataset consists of a series of atomic structures and their corresponding energies, forces, and stresses, and is typically evaluated using electronic structure methods like DFT. In the case of carbon, several peculiarities exist related to its diverse chemical bonding.

The visualization of the training data used for the construction of our carbon ACE parametrization is provided in *(Fig. 4.6)*. The dataset encompasses more than seventeen thousand structures that were chosen to sample a broad range of atomic configurations for carbon to ensure both accuracy and transferability.

Fracture simulations of brittle materials are very challenging as they require transferable models that are able to describe bond-breaking processes under large and inhomogeneous stresses. At the same time, the models need to remain numerically efficient to be able to simulate large supercells with complex crack geometries at finite temperatures and over realistic time scales. We performed MD simulations of brittle cleavage of diamond using ACE and two other machine-learned potentials GAP20 and PANNA to compare the predictions of these three models.

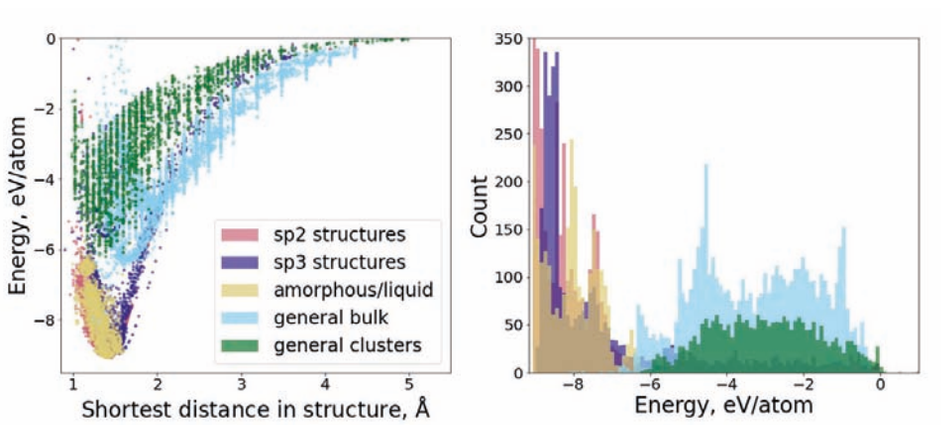


Fig. 4.6: Visualisations of the training dataset in terms of energy per atom with respect to the nearest interatomic distance within each structure (left) and the distribution of cohesive energies (right).

We simulated semi-infinite cracks with periodic boundary conditions applied along the crack front. The atomic configurations were generated by applying a given stress intensity factor K_I to model the asymptotic crack tip region according to linear elastic fracture mechanics. Depending on the magnitude of the applied stress, the crack either tends to heal or propagate during the simulation. Our simulations show that below the critical loading, all models predict the crack to close along the crack plane. However, ACE is the only model that sustains brittle cleavage when the loading exceeds the critical value of about 4.2 MPa $m^{1/2}$, which is in good agreement with experimental observations. In contrast, both GAP20 and PANNA models show local structural transformations into graphitic structures, which lead to blunting the crack tip, as displayed in *(Fig. 4.7)*

The great variability of amorphous carbon (a-C) networks, governed by competing sp, sp^2 and sp^3 hybridizations, poses another difficult challenge for atomistic simulations, and there exist marked differences in the predictions of structural and physical properties of a-C systems from different atomistic models. We studied the properties of bulk a-C samples using large-scale molecular dynamics (MD) simulations. The samples with densities ranging from 1.8 (low-density nanoporous structures) to 3.5 (diamond-like a-C) g/cm^3 were prepared using three different quench rates. Snapshots of representative structures are shown in *(Fig. 4.8)*.

Samples generated with the fast quench rate exhibit uniformly disordered structures that differ mainly in the fraction of the sp^2 and sp^3 bonded atoms. However, at the slow cooling rate, which was only possible to achieve due to the outstanding ACE efficiency, we observe an occurrence of more ordered structures with clearly separated sp^2 and sp^3 regions. For the lower densities, slow quenching leads to extended graphitic sheets with fewer defects. Hence, our simulations demonstrate for the first time a clear influence of the quench rate on the a-C morphology with a non-classical potential.

In summary, our carbon ACE opens new possibilities for the structural modelling of carbon at the atomic scale. It not only describes the fundamental properties of carbon allotropes with DFT accuracy, but is also able to maintain this accuracy in large-scale simulations. If

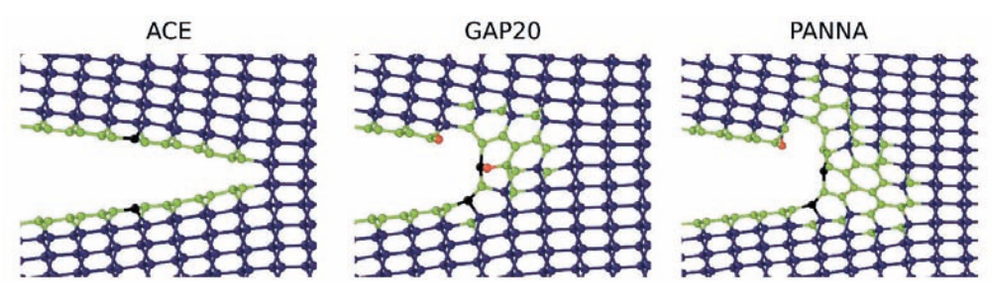


Fig. 4.7: Snapshots of crack configurations above the critical loading predicted by different models. The blue and green coloured atoms correspond to the sp^3 and sp^2 bonding, respectively. GAP20 and PANNA show local structural transformations into graphitic structures at the crack tip while ACE maintains a brittle cleavage.

necessary, the ACE accuracy and transferability can be further improved systematically, either by tailoring the training dataset for the required application or by extending the ACE basis. Finally, the elemental ACE models can be readily extended or combined to address multicomponent systems, such as hydrocarbon systems or transition metal carbides.

M. Qamar, M. Mrovec, Y. Lysogorskiy, A. Bochkarev, and R. Drautz,
Atomic cluster expansion for quantum-accurate large-scale simulations of carbon,
Journal of Chemical Theory and Computation, accepted

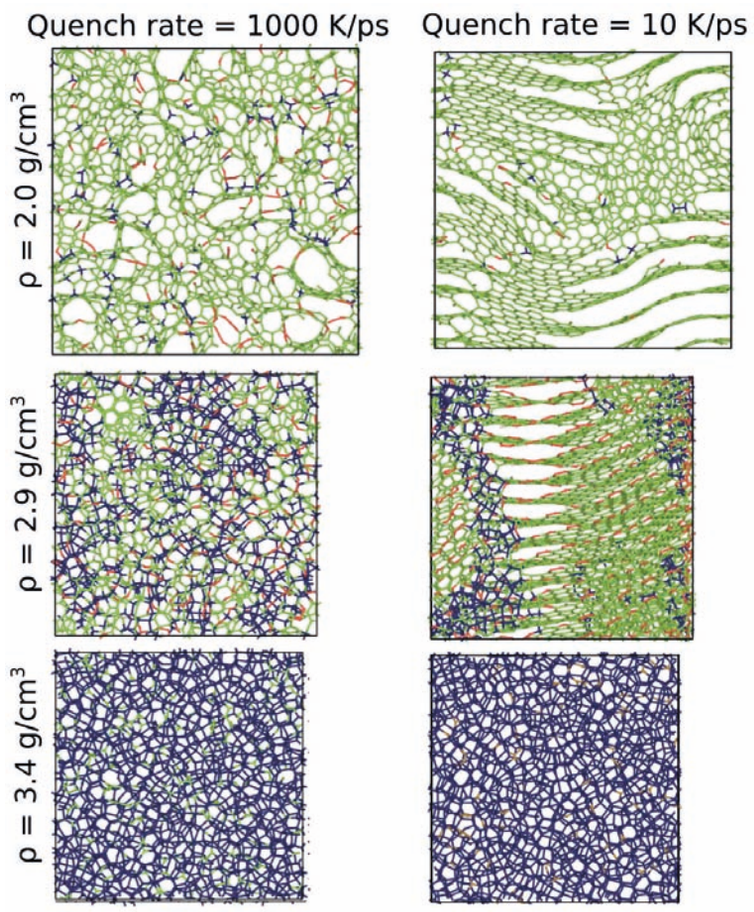


Fig. 4.8: Representative a-C structures of three densities using 1000 K/ps (left) and 10 K/ps (right) quench rates. The slices of 1 nm thickness were cut out of a larger simulation cell. White, red, green, and blue colours correspond to 1-fold, 2-fold, 3-fold, and 4-fold coordinated atoms, respectively.

AMS

4.3. Data-Driven Methods for Atomistic Simulations

Group leader:
Dr. Yury Lysogorskiy

Group members:
Dr. Anton Bochkarev
Eslam Ibrahim
Dr. Matteo Rinaldi

▸ Research

The research group develops and applies data-driven methods in materials science, with a principal emphasis on atomic-scale simulations using the Atomic Cluster Expansion (ACE) – a new type of machine learning interatomic potentials with a formally complete basis set. Our research covers the full cycle of ACE model parameterization and validation: extensions to the formalism, implementation in high-performance simulation codes such as LAMMPS, parameterization of ACE using non-linear optimization with TensorFlow as well as uncertainties indication and active learning strategies. It also includes deploying high-throughput calculations for computing reference data with DFT and workflows for validating interatomic potentials for accuracy and transferability.

▸ Competences

- Atomic Cluster Expansion (ACE): method development, parameterization and validation
- High-throughput calculations (DFT and molecular dynamics)
- Data-driven methods in materials science: machine learning, generative models

Performant implementation of the atomic cluster expansion (PACE): application to copper and silicon

The atomic cluster expansion is a general polynomial expansion of the atomic energy in multi-atom basis functions. We implemented the ACE in the performant C++ code PACE that is suitable for use in large-scale atomistic simulations with LAMMPS[1]. It was demonstrated that the atomic cluster expansion as implemented in PACE shifts a previously established Pareto front for machine learning interatomic potentials [2] toward faster and more accurate calculations. It was also shown that the Cu and Si ACE potentials significantly improve on the best available potentials for highly accurate large-scale atomistic simulations.

[1] Y. Lysogorskiy, C. van der Oord, A. Bochkarev, S. Menon, M. Rinaldi, T. Hammerschmidt, M. Mrovec, A. Thompson, G. Csányi, C. Ortner, R. Drautz,
Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon,
npj Computational Materials, 7, 1-12, 2021

[2] Y. Zuo, C. Chen, X. Li et al.
Performance and cost assessment of machine learning interatomic potentials
Journal of Physical Chemistry A 124, 731–745, 2020

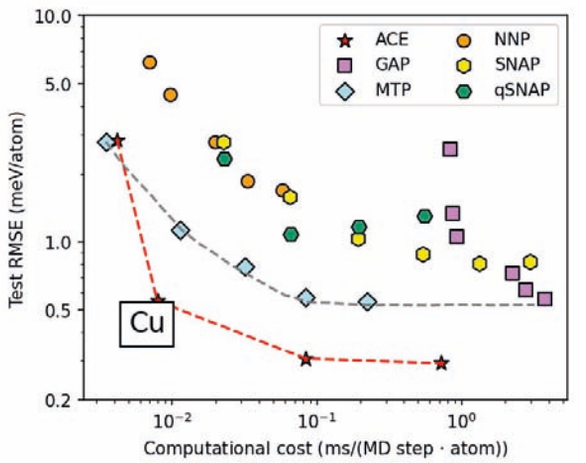


Fig. 4.9: Test root mean square error vs. computational cost for Cu for ACE potentials compared to a recent benchmark study (Zuo et al. 2020). The timings were reduced by constant factors to correct for hardware differences, and the ACE timings then overlaid.

Efficient parametrization of the atomic cluster expansion

It this work, an efficient framework for parametrization of ACE models for elements, alloys, and molecules was presented. To this end, first general requirements for a physically meaningful description of the atomic interaction was introduced in addition to the usual equivariance requirements.

It was demonstrated that ACE can be converged systematically with respect to two fundamental characteristics - the number and complexity of basis functions and the choice of nonlinear representation. The construction of ACE parametrizations is illustrated for several representative examples with different bond chemistries, including metallic copper, covalent carbon, and several multicomponent molecular and alloy systems.

Our ACE parametrization strategy is implemented in the freely available software package pacemaker, which enables largely automated and GPU-accelerated training. The resulting ACE models are shown to be superior or comparable to the best currently available ML potentials and can be readily used in large-scale atomistic simulations.

A. Bochkarev, Y. Lysogorskiy, S. Menon, M. Qamar, M. Mrovec, R. Drautz,
Efficient parametrization of the atomic cluster expansion,
Physical Review Materials, 6, 013804, 2022

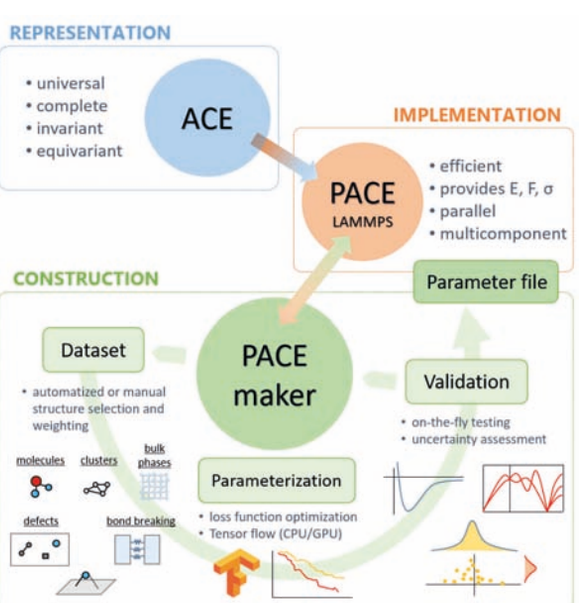


Fig. 4.10: Block scheme of the main pacemaker workflow.

Multilayer atomic cluster expansion for semi-local interactions

Traditionally, interatomic potentials assume local bond formation supplemented by long-range electrostatic interactions when necessary. This ignores intermediate-range multiatom interactions arising from the relaxation of the electronic structure. The multilayer atomic cluster expansion (ml-ACE) was presented, which includes collective, semi-local multiatom interactions naturally within its remit. It was demonstrated that ml-ACE significantly improves fit accuracy and efficiency compared to a local expansion on selected examples and provides physical intuition to understand this improvement.

A. Bochkarev, Y. Lysogorskiy, C. Ortner, G. Csányi, R. Drautz,
Multilayer atomic cluster expansion for semi-local interactions,
Physical Review Research 4, L042019, 2022

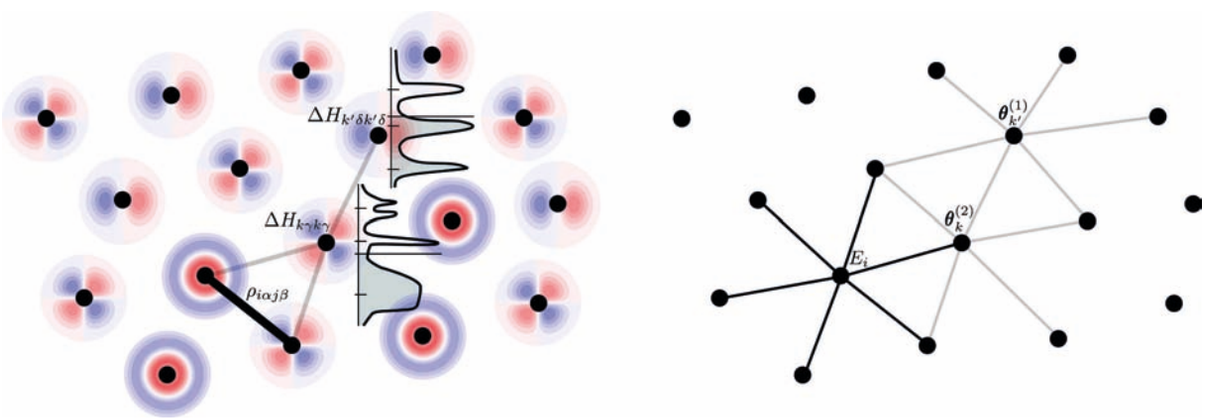


Fig. 4.11: Semi-local interactions in electronic structure calculations. Changes in the onsite levels are a function of the local environment that depends on the onsite levels of further distant atoms (left). Abstraction in multilayer-ACE. The energy E_i of atom i depends on state of neighboring atoms through indicator field $\theta^{(2)}_{k'}$ on atom k that depends on further indicator fields $\theta^{(2)}_{k'}$ (right).

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. In addition, finite element methods are used, e.g., to predict damage processes in biological tissues.

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 (the electronic versions Open Access); the compilation was co-authored by me and the research assistant Hesham Salama, who organized the tutorial sessions in the last years.

▸ 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)

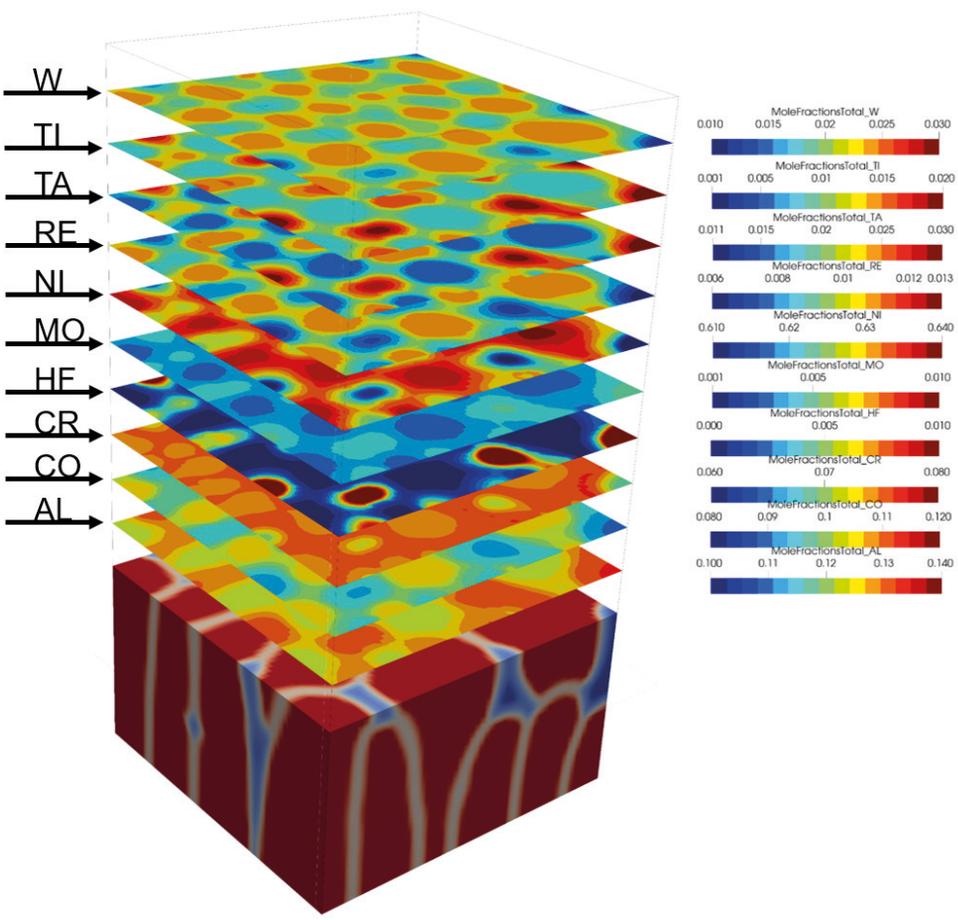


Fig. 5.1: Solidification under additive manufacturing conditions: Simulation with full complexity at 10 component CMSX4 (Murali Uddagiri 2023, unpublished)

STKS

5.1. Phase-Field Simulations of Microstructures

Group leader:
Dr. Oleg Shchyglo

Group members:
Muhammad Adil Ali
Dr. Hossein Jafarzadeh
Hesham Fathy Mohamed Ali Salama
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

Modeling of divorced eutectic microstructure

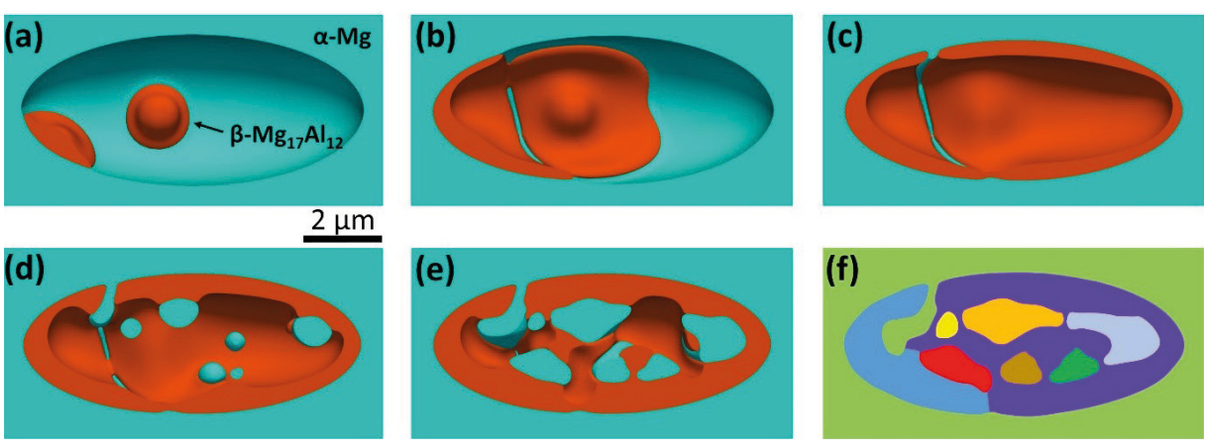


Fig. 5.2: Nucleation and growth of the β phase in the liquid pocket near the eutectic temperature followed by the nucleation and growth of the α phase in the residual liquid.

In this study, the partially divorced eutectic microstructure of α-Mg and β-$Mg_{17}Al_{12}$ was investigated by electron backscatter diffraction, transmission electron microscopy, and phase-field modeling in hypoeutectic Mg-Al alloys. The orientation relationships between the individual eutectic α grains, the eutectic β phase, and the primary α grains were investigated. While the amount of eutectic morphology is primarily determined by the Al content, the in-depth microstructure analyses and the phase-field simulation suggest non-interactive nucleation and growth of the eutectic α phase in the β phase grown on the interdendritic primary α dendrites. Also, phase-field simulations showed a preferred nucleation sequence, where the β phase nucleates first and subsequently triggers the nucleation of the eutectic α phase at the moving β phase solidification front, which supports the microstructural analysis results.

J.-H. Kang, J. Park, K. Song, C.-S. Oh, O. Shchyglo, I. Steinbach,
Microstructure analyses and phase-field simulation of partially divorced eutectic solidification in hypoeutectic Mg-Al alloys,
Journal of Magnesium and Alloys, 10, 1672-1679, 2022

Phase-field simulation of creep in superalloys

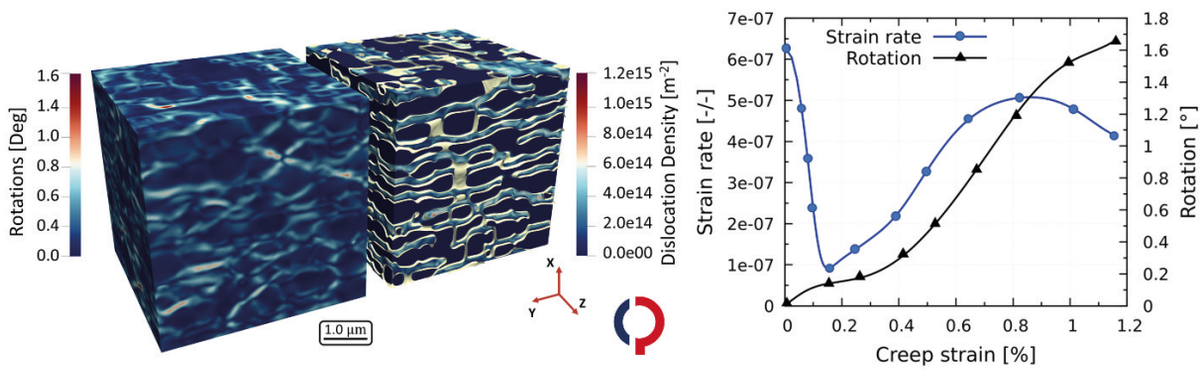


Fig. 5.3: Spatial distributions of rotation angles and dislocation density in the microstructure of a Ni-based superalloy at 1% creep strain under external uniaxial tension.

A dislocation density-based crystal plasticity—phase-field model is applied to investigate directional coarsening during creep in CMSX-4 Ni-based superalloys in the high-temperature and low-stress regime. Coherency between the ordered γ' precipitates and the disordered γ channels prevents the generation of geometrically necessary dislocations, since the precipitate can be considered undeformable in the low stress regime. After coherency loss between the γ matrix phase and the γ' precipitates the constraint against generation of geometrically necessary dislocations is relaxed, causing rotation of the crystal lattice under uniaxial load, known as "Schmid rotation". As a consequence, the creep rate in the matrix increases, whereby degradation can be measured by the number density of geometrically necessary dislocations. The state of coherency loss is associated with the minimum creep rate in a creep experiment under constant load. The presented simulations start from a coherent γ' precipitates distribution with random size and position, generated during a precipitation heat treatment process. Simulations of N-type and P-type rafting under tensile and compressive load respectively are presented. The effect of coherency loss, coalescence of precipitates and lattice rotation due to the generation of geometrically necessary dislocations is discussed in correlation with experimental findings.

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

Phase-field study of additive manufacturing of Ni-based superalloys

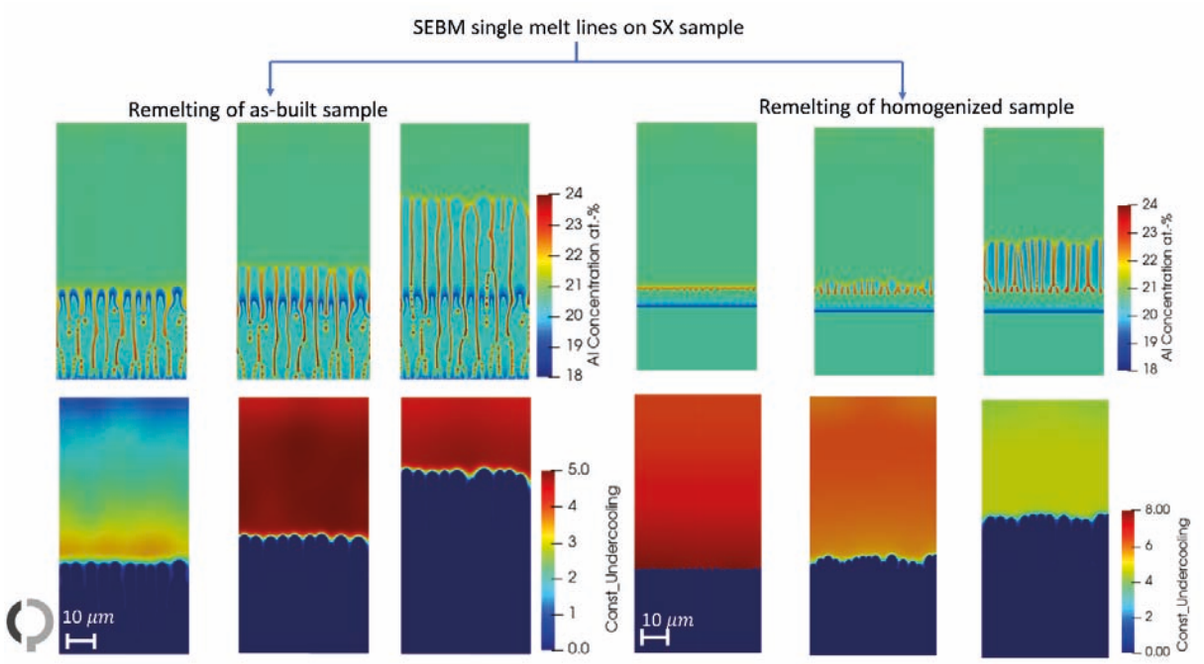


Fig. 5.4: Evolution of composition and constitutional undercooling during partial remelting of as-built (left) and homogenized (right) single crystal (SX) sample of Ni-Al binary alloy system.

In the current work, we employ multi-phase-field simulations to understand the effect of remelting on microstructure evolution, especially on nucleation of new grains during selective electron beam melting (SEBM) of Ni-based superalloy. The phase-field model is coupled to both mass and heat transport phenomena including the release of latent heat of solidification. We run remelting simulations in both as-cast and homogenized conditions. Experimental observations show that remelting triggers the nucleation of new grains at the melt-pool border. The simulation results shed more light on the local conditions at the melt-pool border thereby enhancing our understanding of the mechanisms responsible for the nucleation. The simulation results are validated with experimental results obtained for the Ni-20.5 %Al model binary alloy.

M. Uddagiri, O. Shchyglo, I. Steinbach, B. Wahlmann, C. Koerner,
Phase-field study of the history-effect of remelted microstructures on nucleation during additive manufacturing of Ni-based superalloys,
Metallurgical and Materials Transactions A (2023) DOI: 10.1007/s11661-023-07004-0

STKS

5.2. Theory and Simulation of Complex Fluids

Group leader:
Prof. Dr. Fathollah Varnik

Group members:
Reza Namdar
Mohammad Norouzi

▸ Research

The research interest of the complex fluids group includes various physical phenomena in fluidic environments. Two examples from the group's recent activity are hemodynamics of blood flow through aneurysms, and heat-exchange in flows through packed arrangements of solid bodies. In studying blood flow through constrictions and aneurysms, the group uses a hybrid numerical tool based on a combination of the lattice Boltzmann method as fluid dynamics solver with the finite element approach to update the dynamics of blood vessel and particular objects such as red blood cells. For the study of combustion phenomena in flows through packed beds, a modified version of the lattice Boltzmann method has been adapted which allows accounting for large changes of fluid density due to local heating, which arises from chemical reactions. Here, the group is also conducting fundamental theoretical work and is establishing the connection between macroscopic equations, which govern the change of species mass due to chemical reactions, energy production and mass and heat transport, on the one hand, and diffuse interface methods such as the phase field approach, on the other hand. As to the study of amorphous materials, molecular dynamics simulations are used to address the shape memory effect in polymers and the connection between the structure and the mechanical properties (e.g., ductility) in bulk metallic glasses. The work of the complex fluids groups is being almost always performed in collaboration with other partners to take advantage of their complementary expertise. Some examples here are the study of tissue degradation in aneurysms (D. Balzani, Institute of Mechanics, RUB), work on the ways to improve ductility in metallic glasses (G. Wilde, Institute of Materials Physics, University of Münster), study of additive effects on recovery processes in shape memory polymers (G. Eggeler, Institute of Materials, RUB), and numerical simulations of heat transfer in packed beds (Dominique Thévenin, Otto-von-Guericke-University, Magdeburg, and Benoît Fond, ONERA, Paris).

▸ 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

Improved ductility in metallic glasses via cryogenic cycling

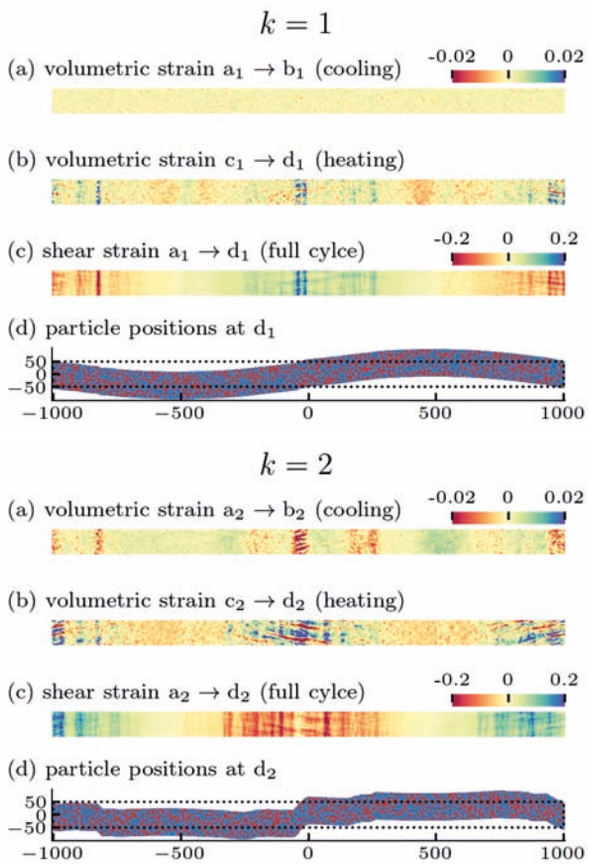


Fig. 5.5: (k=1): Local volumetric strain obtained in the cooling (a1→ b1, panel (a)) and heating (c1→d1, panel (b)) steps of the first thermal cycle. Panel (c) shows the shear strain accumulated over the course of an entire cycle (a1→ d1). Panel (d) shows particle positions projected onto the xz-plane at the time t(d1). In panel (d), the two particle types present in the system are colored in blue and red, respectively. As seen from panel (a), the very first cooling stage leads to a rather homogeneous distribution of local expansion/contraction. During the subsequent heating, (c1→d1, panel (b)), a heterogeneous deformation field is observed with a clear signature of strain-localization. This is also visible in panel (c), where shear strain is localized in multiple shear bands. A closer look at panel (d) reveals kinks roughly at the same x-positions, where the shear bands in (c) occur. These kinks gradually fill the system as cryogenic cycling goes on. (k=2): The same date as for (k=1) but now for the second thermal cycle. Compared to the first cycle, a heterogeneous response to the temperature change is well pronounced already in the cooling stage (a2→b2, panel (a)) with a sequence of contracting (red) and expanding (blue) regions. Interestingly, domains where bands of negative volumetric strain (contraction) appear in this cycle coincide with the regions where shear-strain-localization is observed in the first cycle. Localization of volumetric strain is also visible in the heating stage (c2→d2, panel (b)). As to the shear-strain (panel c), we again find the clear signature of localization in bands similar to k = 1. The overall deformation of the sample in panel (d) now shows a larger number of kinks as compared to the first cycle. The images are taken from Bruns and Varnik, J. Chem. Phys. 156, 234501 (2022).

Despite their remarkable mechanical properties such as large elastic modulus and high toughness, bulk metallic glasses have still not made their way to widespread use as structural components. The main obstacle here is low deformability and brittle fracture. An important research focus has thus been on new mechanical and thermal processing procedures with the aim of improving the ductility of bulk metallic glasses. Along this line, it has been recently proposed that thermal cycling between a cryogenic temperature (a temperature well below the glass transition point of the material) and the operating temperature could improve fracture limit and ductility in metallic glasses. We have investigated this issue via molecular dynamics simulations of a generic molecular glass model and have found that the occurrence of such an effect depends both on the process parameters such as the selected temperature interval and the rate of cooling and reheating as well as on the degree of structural heterogeneity in the material, the latter being influenced by the ageing process prior to thermal treatment. Most importantly, our simulations provide direct atomistic evidence for a raise in the visited energy landscape, which can be also interpreted as a sign of improved ductility. These conclusions are in line with recent results obtained from mechanical investigations of the degree of brittleness.

M. Bruns, F. Varnik,
Enhanced dynamics in deep thermal cycling of a model glass,
The Journal of Chemical Physics 156, 234501, 2022

Additive effects on shape memory polymers

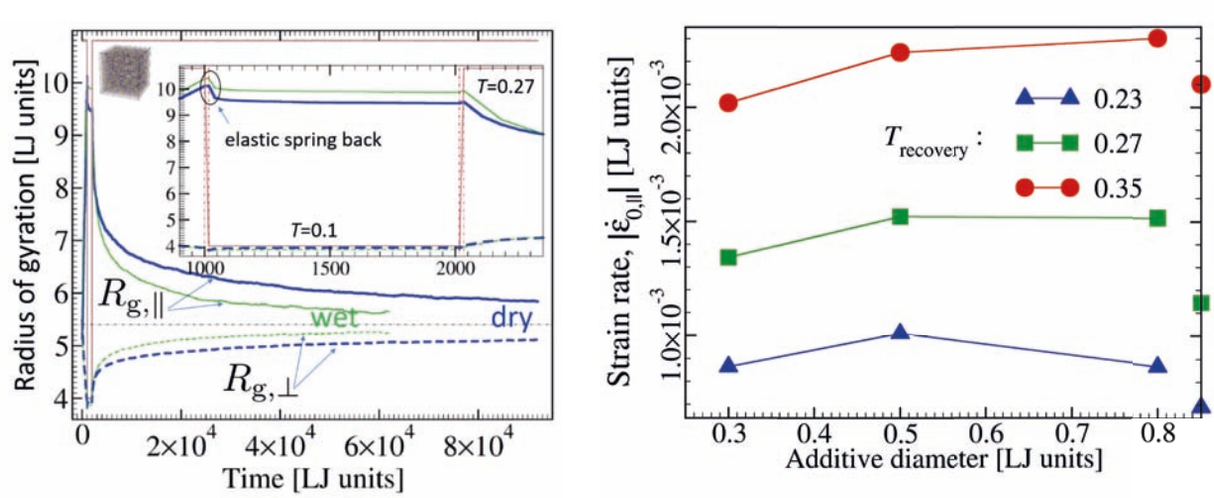


Fig. 5.6: Chain deformation and effect of additive molecules on recovery in a model shape memory polymer. Components of chains' gyration tensor parallel (solid lines) and perpendicular (dashed lines) to the direction of deformation during a shape memory cycle. Thick blue lines correspond to a dry sample and green lines to a probe with a 20% concentration of spherical particles. The inset zooms in the late stage of deformation until the beginning of recovery. (b) The rate of strain recovery versus additive diameter at three different recovery temperatures (concentration=20%). The data for T=0.23 (< T_g ≈0.25) shows a maximum for an additive diameter roughly equal to half of the monomer size (note that the latter is used as the unit of length). All quantities are given in the reduced Lennard-Jones units. The images (adapted) are taken from Zirdehi et al, Materials 10,327 (2021).

The role of conformational degrees of freedom for the one-way effect in shape memory polymers is directly evidenced via molecular dynamics simulations. A study of the statistical average of the gyration tensor, projected onto two distinct directions, parallel and perpendicular to uniaxial deformation, clearly shows that chains are stretched during the deformation stage (parallel component of the gyration tensor increases and the normal one decreases). Below the glass transition temperature T_g, polymer chains are frozen and therefore cannot explore the conformation space. As a result, they remain in a stretched state. When the system is re-heated, the macromolecules become mobile and can relax. This is best visible in the two principal components of the gyration tensor, which now approach each other, demonstrating the striving of the system towards higher entropy. Most importantly, the entire sample starts to recover its original shape simultaneously with this chain relaxation process. Relaxation of conformational degrees of freedom is thus the main cause of shape recovery. Moreover, data on the effect of the chemical environment reveal that, in line with experimental findings, a sample containing additive particles exhibits a faster recovery than an additive-free one.

E. M. Zirdehi, H. Dumlu, G. Eggeler, F. Varnik,
On the size effect of additives in amorphous shape memory polymers,
Materials 10,14(2):327, 2021

Tissue degradation in cerebral aneurysms

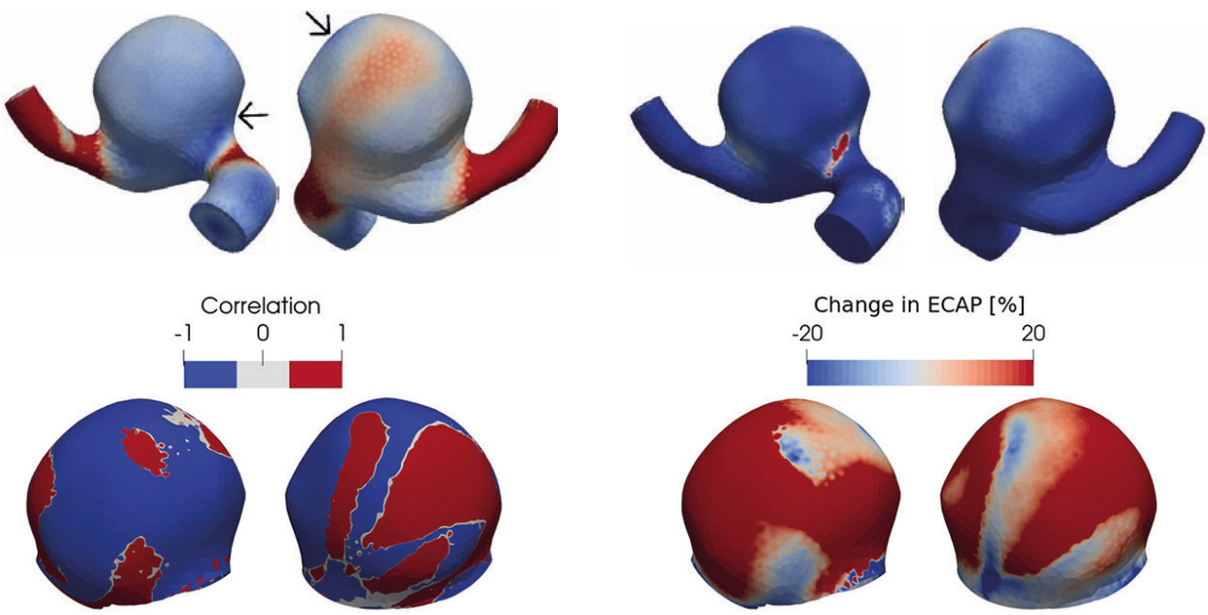


Fig. 5.7: Time-averaged wall shear stress (WSS) (the two top-left images) and oscillatory shear index (OSI) (the two top-right images) fields in the presence of degradation for a patient-specific aneurysm geometry (C0034 in Aneurisk dataset repository (Aneurisk-Team, 2012). The two images on the bottom left show degradation-induced relative changes in WSS and OSI. The remaining two images (bottom right) depict the corresponding changes in endothelial cell activation potential (ECAP).

In the context of degradation of blood vessel tissues in an aneurysm, numerical studies of blood flow through an aneurysm reveal an interesting connection between tissue degradation and variations of the (time-averaged) wall shear stress (WSS), i.e., tangential forces acting on tissue wall, and the so-called oscillatory shear index (OSI), which is a measure of stress variations with time. We find that, at certain areas of an aneurysm sac, WSS is reduced while at the same time OSI is enhanced during degradation. Since this feature is stronger at places with low wall shear stress, it may have important implications for the further evolution of tissue degradation. Indeed, prior observations suggest that a low wall shear stress may stimulate tissue degradation. When combining with this fact, our numerical simulation results thus suggest that at sites where OSI accompanies a low WSS a degradation-loop may occur: Degradation of an aneurysm wall can lead to lower wall shear stress and higher oscillatory shear index, which correspond to a favorable environment for pathological changes such as atherosclerosis and thrombus formation in the aneurysm. Such a flow environment, in turn, may induce further degradation.

H. Wang, K. Uhlmann, D. Balzani, V. Vidula, F. Varnik
On the potential self-amplification of aneurysms due to tissue degradation and blood flow revealed from FSI simulations,
Frontiers in Physiology, 12, 785780, 2021

STKS

5.3. Diffusion in Metals and Minerals

Group leader:
Dr. Julia Kundin

Group members:
Ahmadreza Riyahi Khorasgani

▸ 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 ifferent 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

Understanding diffusion in multiprincipal element systems

Tracer diffusion coefficients along the diffusion path in diffusion couple $Co_{17}Cr_{20}Fe_{20}Mn_{20}Ni_{23}/Co_{23}Cr_{20}Fe_{20}Mn_{20}Ni_{17}$ were measured. The experimental tracer diffusion coefficients are consistent with the mobility database produced in the previous studies. The diffusion couple's chemical and tracer concentration profiles are reproduced with the thermo-kinetic database developed by using the PyMob software. The intrinsic and interdiffusion coefficients for multicomponent alloys were estimated. Moreover, recent advances in the field of diffusion in multiprincipal element systems were critically reviewed, with an emphasis on experimental as well as theoretical approaches to determining atomic mobilities (tracer diffusion coefficients) in chemically complex multicomponent systems.

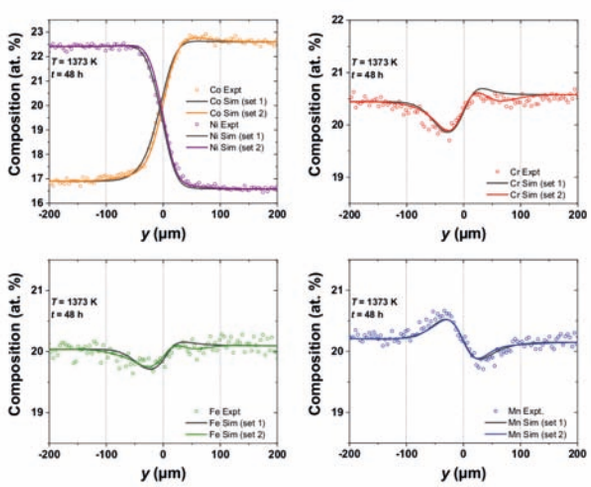


Fig. 5.8: Comparison between the experimentally measured and simulated interdiffusion profiles in Co_{17}-Ni/Co_{23}-Ni diffusion couple at 1373 K after 48 h.

D. Gaertner, J. Kundin, I. Steinbach, S. V. Divinski, et al.,
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

A. Dash, A. Paul, S. Sen, S. V. Divinski, J. Kundin, I. Steinbach, B. Grabowski, X. Zhang,
Recent advances in understanding diffusion in multiprincipal element systems,
Annual Review of Materials Research, 52, 383-409, 2022

Modeling the non-equilibrium vacancy diffusion

In order to understand the influence of the vacancy fluxes on the assessment of the diffusion coefficients, the simulation of the interdiffusion with vacancy flux will be carried out on an example of the HEA alloys, in particular for the CrFeNi system. A practical thermodynamically based model of multi-component diffusion with non-equilibrium vacancies has been developed. We study the effect of the chemical potential gradient of vacancies, i.e. vacancy gradient on the pore fractions, the diffusion of vacancies for different cases of sink/source intensity, and the effect of the vacancy formation energy on diffusion through the thermodynamic factor and equilibrium vacancy concentration.

C.-H. Xia, J. Kundin, I. Steinbach, S. V. Divinski,
Model for non-equilibrium vacancy diffusion applied to study the Kirkendall effect in high-entropy alloys,
Acta Materialia, 232, 117966, 2022

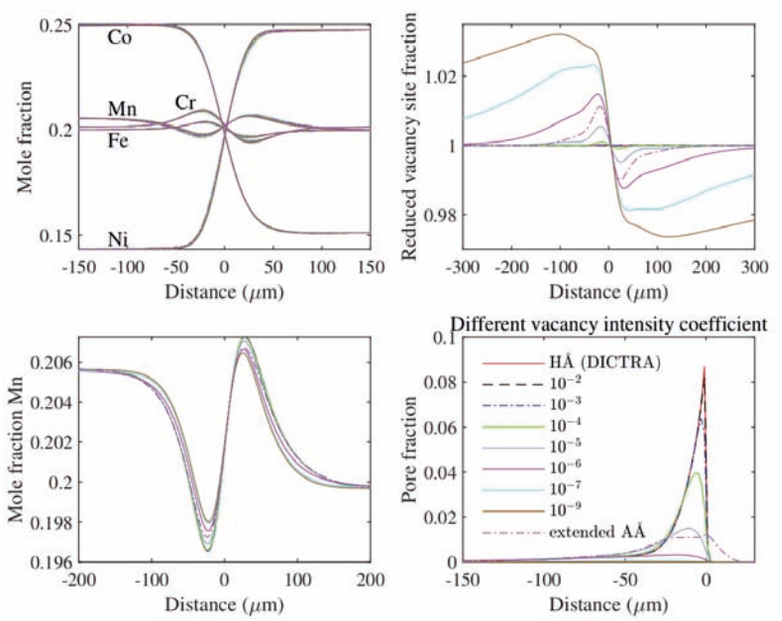


Fig. 5.9: Simulation results of the HEA couple annealed at 1373 K for 48 h by the model of the multi-component diffusion with vacancies: the composition profiles of substitutional components; the reduced site fraction of vacancies; the composition profiles of Mn; the predicted maximum pore fraction.

Developing the automated assessment softwarefor atomic mobility parameters

We developed and improved the PyMob software and hereby have established the kinetic database for HEA alloys. This database together with the thermodynamic databases was checked by the simulation of diffusion couple experiments. The PyMob software combines the CALPHAD method with machine learning methods. The established database for mobility parameters uses as input data the tracer diffusion mobilities obtained by means of the diffusion couple experiments. This is the contribution to the generation of extensive mobility databases for technological applications.

A. Riyahi khorasgani, J. Kundin, S. V. Divinski, I. Steinbach, Reassessment of mobility parameters for Cantor high entropy alloys through an automated procedure, CALPHAD Journal, 79, 102498, 2022

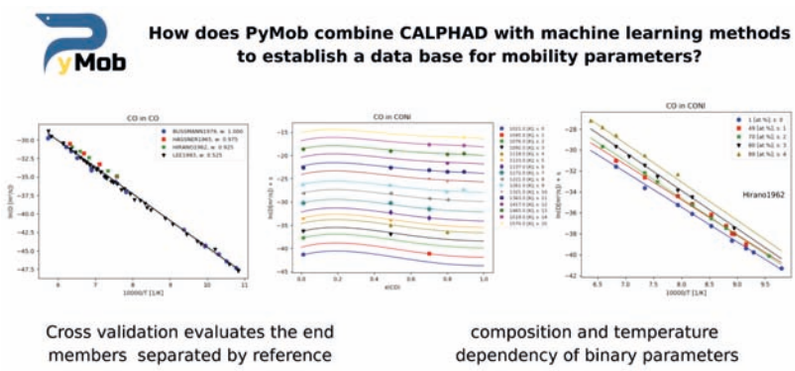


Fig. 5.10: How does PyMob combine CALPHAD with machine learning methods to establish a data base for mobility parameters?

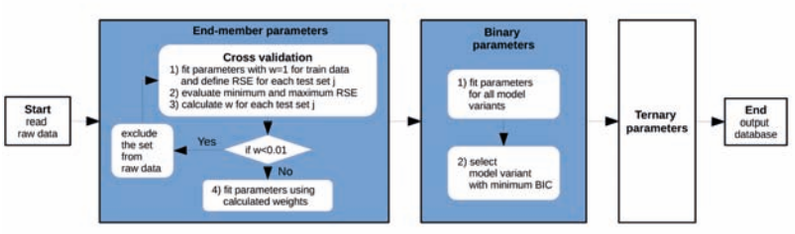


Fig. 5.11: Algorithm of the PyMod software.

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 research focus of the department Micromechanical and Macroscopic Modeling is to gain new insights into the microstructure-property relationships of technologically relevant materials by using the methods of scale-bridging materials modeling. One of our goals is to deepen our understanding of fundamental deformation and failure mechanisms of materials and to predict their macroscopic mechanical properties, which requires scale-bridging modeling since these mechanisms and properties strongly depend on the atomic and the microstructure of materials. With respect to macroscopic mechanical properties, strength under monotonic and cyclic loading, hardness, and fracture toughness are studied 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 the 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 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 modeling.

3. **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.

4. **Data-oriented material modeling:** 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.

The first research area is represented in the group "Fatigue and Fracture Modelling" that was headed by Dr. Mahdieh Shahmardani from April 2020 to

December 2022. Dr. Shahmardani left ICAMS at the end of 2022, and we sincerely thank her for the important contributions to our research in the field of high-temperature and thermomechanical fatigue.

The second research area is supervised by Dr. Hafiz Muhammad Sajjad, and the activities on atomistic modelling within the department MMM are conducted in the group "Mechanical Properties of Interfaces" headed by Dr. Rebecca Janisch.

Finally, Prof. Alexander Hartmaier oversees the research topic "Data-oriented Materials Modeling".

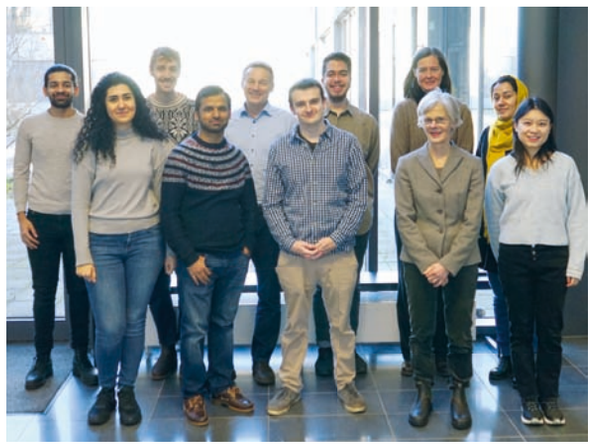


Fig. 6.1: Members of the MMM department at the end of 2022. From left to right: Bilawal Mushtaq, Ronak Shoghi, Jan Schmidt, Hafiz Muhammad Sajjad, Alexander Hartmaier, Timo Schmalofski, Onur Can Sen, Rebecca Janisch, Eva Masuch, Mahdieh Shahmardani, Yunnan Jiang.

The characterization of three-dimensional (3D) microstructures that captures the essential features of a given material is oftentimes desirable for determining critical mechanisms of deformation and failure and for conducting computational modeling to predict the material's behavior under thermo-mechanical loading conditions. However, acquiring 3D microstructure representations is costly and time-consuming because standard microscopic procedures can only produce 2D surface maps. To overcome this problem, we currently investigate possible workflows to generate synthetic 3D microstructures purely from 2D maps of three orthogonal surfaces. The generated 3D microstructures are required to resemble real ones in a statistical sense. To accomplish this, an inverse procedure is established that generates synthetic 3D microstructures with arbitrary microstructure parameters and then compares the surface maps gained from these synthetic microstructures with those obtained from the real materials. In an iterative procedure, the parameters of the microstructure generator are optimized until the best possible agreement between the corresponding surface maps of synthetic and real microstructures is achieved. In this way, the statistical descriptors of the real microstructure are gained as they are represented by the converged input parameters for the microstructure generator. This allows generating different realizations of statistically equivalent 3D microstructures and also varying individual microstructural features in a systematic way to understand their correlation with the mechanical properties of the material.

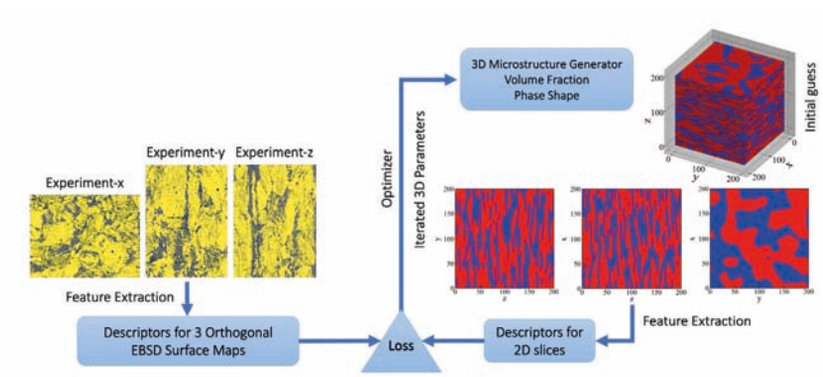


Fig. 6.2: Representation of workflow to reconstruct 3D microstructures from surface maps. The input is represented by three EBSD maps from orthogonal surfaces of a dual-phase steel (yellow: austenite, blue: martensite), from which a low-dimensional, yet representative vector of descriptors is extracted. Corresponding descriptors are generated from a synthetic 3D microstructure (red: austenite, blue: martensite) such that a scalar loss function can be evaluated to assess the degree of similarity of the surface maps of real and synthetic microstructures. In an iterative procedure, the parameters of the 3D microstructure generator are optimized such that the loss function becomes minimal.

MMM

6.1. Fatigue and Fracture Modelling

Group leader (until December 2022):
Dr. Mahdieh Shahmardani

▸ Research

Intermittent mechanical loads combined with high temperatures appear during the operation of turbines in jet engines or in power plants, which can lead to high-temperature fatigue or to thermomechanical fatigue (TMF). Since the assessment of fatigue properties is a complex and time-consuming process, it is essential to develop validated material models that are capable of predicting fatigue behavior, thus allowing the extrapolation of experimental results into a broader range of thermomechanical conditions. To accomplish this, two representative volume elements (RVEs), mimicking the typical microstructure of single crystal Ni-based superalloys and polycrystalline austenitic steels, respectively, are introduced. With the help of these RVEs, the temperature and deformation-dependent internal stresses in the microstructure can be taken into account to predict the macroscopic material behavior. Additionally, phenomenological crystal plasticity models are implemented and parameterized for cyclic deformation of these two materials, thus providing a complete platform to simulate the material response under different mechanical and thermal loads.

The most important conclusion from the comparison of the isothermal fatigue behavior of the two different materials is that the kinematic hardening, which determines the cyclic plasticity of the materials and is responsible for the shape of the hysteresis loops, is entirely described by the internal stresses within the typical microstructure of the Ni-based superalloy, which is modeled in a scale-bridging approach. Hence, no additional terms for kinematic hardening need to be introduced to describe the cyclic plasticity in the superalloy. For the austenitic steel, in contrast, the Ohno-Wang model for kinematic hardening needs to be considered additionally to the internal stresses in the polycrystalline microstructure to obtain a correct description of its cyclic plasticity.

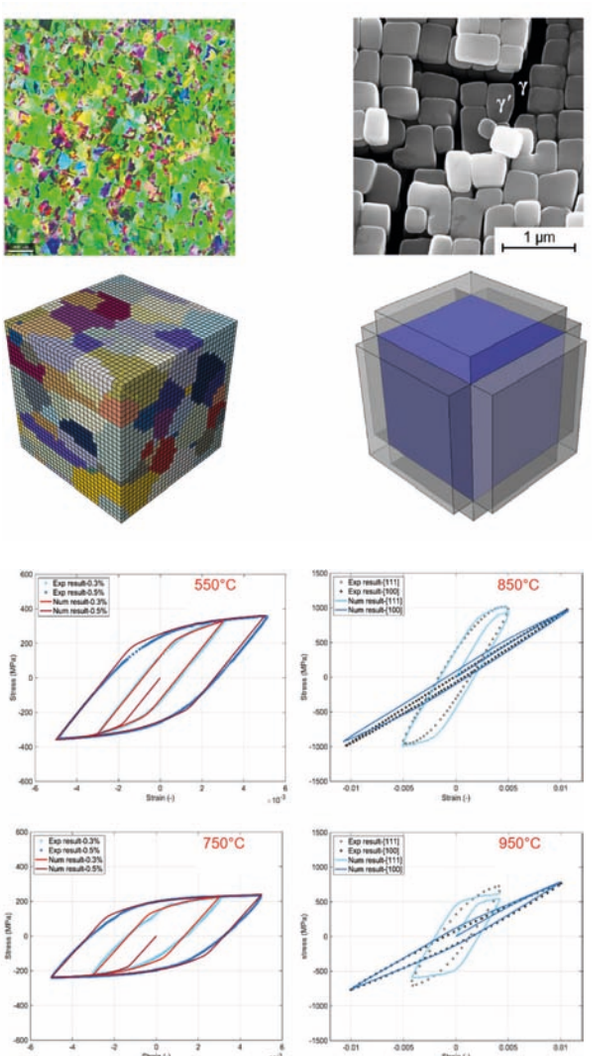


Fig. 6.3: Microstructures of austenitic steel from additive manufacturing and from nickel-based superalloys, respectively; the derived Representative Volume Elements (RVEs) form the basis of micromechanical simulations of uniaxial fatigue loading at different temperatures, which are compared with experimental data.

MMM

6.2. Mechanical Properties of Interfaces

Group leader:
PD Dr. habil. Rebecca Janisch

Group members:
Timo Klaus Schmalofski
Onur Can Sen

► Research

The focus of the research group "Mechanical Properties of Interfaces" lies on the fundamental processes occurring at interfaces, which strongly affect the strength and deformability of polycrystalline microstructures in metals and alloys, and their relation to the atomistic structure of the internal boundaries.

These processes are investigated by means of atomistic simulations. Ab-initio electronic structure calculations based on density functional theory are used to predict the energy, strength, and effective modulus of interfaces and other defects in iron and ferritic steel. Such characteristic properties are used to identify and understand trends, e. g.~on hydrogen solubility in ferritic microstructures and on its effect on grain boundary cohesion. Thus, guidelines for alloy design and constitutive relationships for multiscale simulations, e.g. of hydrogen-enhanced decohesion, are derived. A combination of atomistic methods with a statistical assessment of the parameter space that defines the structure of grain boundaries allows a larger survey of structures in an efficient manner, which is needed to derive structure-property relationships.

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

In 2021/2022 the group's projects focused on the role of the excess volume of grain boundaries for the solution of H, the development of an efficient algorithm that combines design of experiment principles with atomistic simulations and the role of defects and crack geometry during fracture of lamellar and polycrystalline TiAl microstructures

► Competences

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

Atomistics meets statistics – an efficient sampling of the grain boundary parameter space

High-throughput numerical simulations are frequently used in materials development because they allow a systematic variation of material or process parameters. The most common approach to cover a broad range of these parameters in a short time is based on a regular, i.e., equidistant sampling of the parameter space, which keeps the automatization of the workflow simple. It has limited use, however, when the properties of interest depend on several variables at the same time, i.e., a multidimensional parameter space has to be sampled, and the property of interest does not vary homogeneously in this space. This is the case for the energy of grain boundaries, which depends on the five macroscopic geometric degrees of the interface freedom, defined by the rotation axis and angle and the inclination of the grain boundary plane, and which exhibits deep local minima, so-called cusps.

For this purpose, a sequential design of experiment (DOE) algorithm was developed, in which the next points to be sampled are chosen based on the already available data. The algorithm is outlined in (*Fig. 6.4*). After creating a first set of structure-energy data with atomistic simulations, the so-called Kriging predicts the value of a function at given interpolation points. It is related to a Gaussian regression analysis and provides a natural measure of uncertainty for predictions at potential locations. In the sequential design, this information is used to create a list of candidate points for new sampling locations from the regions where the uncertainty is maximal via the jackknife method. In these regions the points with the maximum expected variance compared to their neighbours will be chosen, in other words, points which are expected to be on a steep slope in the energy landscape. The main advantage of this sequential design is that cusps which are not included in the initial data are identified by the algorithm after a few steps only. This is particularly advantageous for more complex subsections of the 5D parameter space, such as the energy as a function of boundary plane inclination, shown for the example of a [110] 7.5 small angle grain boundary. The underlying strategy can be adapted for any application with strong, localized fluctuations in the values of the unknown function.

M. Kroll, T. Schmalofski, H. Dette R. Janisch, Efficient Prediction of Grain Boundary Energies from Atomistic Simulations via Sequential Design, Advanced Theory and Simulation, 2100615, 2022

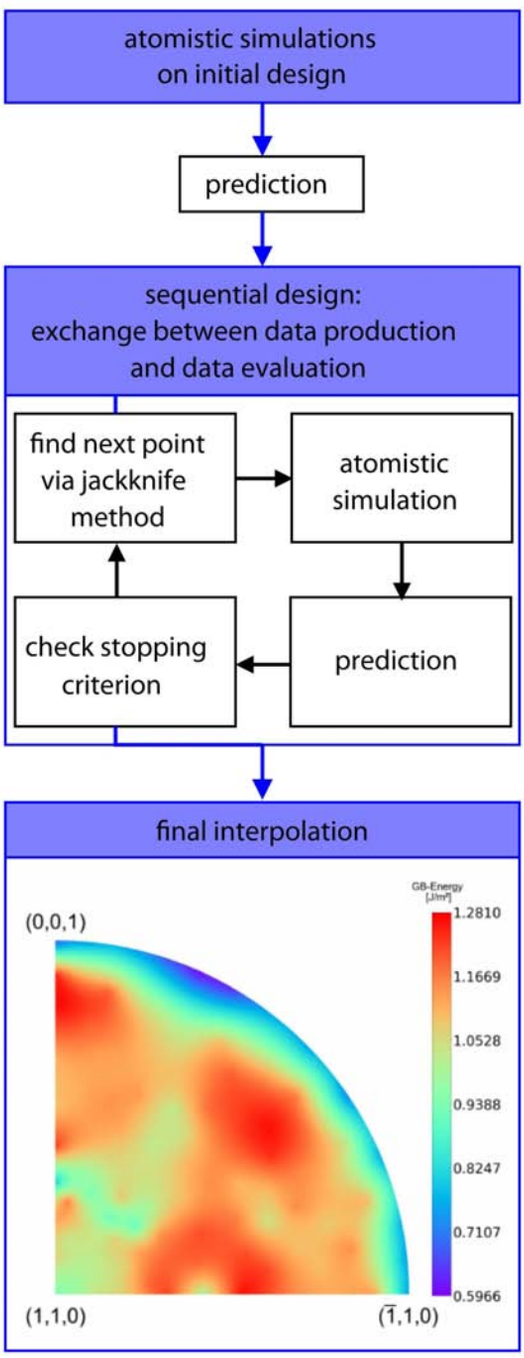


Fig. 6.4: Flowchart of the algorithm to sample grain boundary energies, consisting of initial design, sequential design and final Kriging interpolation. The example shown for the final interpolation is the energy in the fundamental zone of grain boundary inclinations for a [110] 7.5° grain boundary in fcc Ni.

Lamellar size-dependent fracture behavior of γ -TiAl

Strengthening of metals by incorporating nanoscale coherent twin boundaries is one of the important breakthroughs of recent years in overcoming the strength-ductility trade-off. To this effect, also twin boundaries in nanolamellar lightweight Ti-Al alloys promise great potential, but their contribution to the deformation and fracture behavior needs to be better understood for designing optimal microstructures. Via a series of large-scale molecular statics simulations, it was analyzed how far and how exactly the lamellar size λ controls the onset and fracture along true twin boundaries in fully lamellar γ -TiAl. The principle of the setup is shown in (*Fig.6.5*). It is observed that even at the nanoscale, the fracture initiation toughness increases with decreasing λ in a somewhat linear fashion with $\lambda^{-1/2}$, i.e., in the style of a classical Hall-Petch type relation, see (*Fig.6.6*). This relation breaks down below 3.04 nm lamella thickness; at smaller λ an inverse Hall-Petch type behavior occurs. In addition, the actual crack tip mechanisms are sensitive to λ as well: Larger λ facilitate dislocation mediated crack tip plasticity and gradual blunting of the crack tip, while crack tip deviation and brittle fracture are more favorable for thinner lamellae, in the range below 3 nm. This means that there is a brittle-to-ductile transition for a critical lamella thickness in the region between 1.64 and 3.04 nm, above which the crack tip events are primarily dislocation-based plasticity and below which cracks propagate in a quasi-brittle manner.

A. Neogi, R. Janisch,
Unravelling the lamellar size-dependent fracture behavior of fully lamellar intermetallic γ –TiAl,
Acta Materialia 227, 117698, 2022

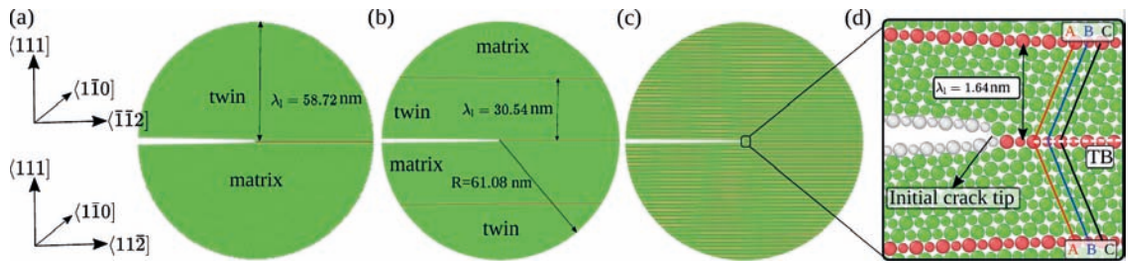


Fig. 6.5: Examples of atomistic configurations of initial pre-cracked γ /γ lamellar geometries with different lamellar sizes (a-c), and (d) a close-up of the crack tip region. Ti and Al atoms are represented by bigger and smaller balls. Atoms are colored based on the common neighbor analysis: fcc - green, hcp - red, and surface atoms - white. Reprinted from [Neogi et al.].

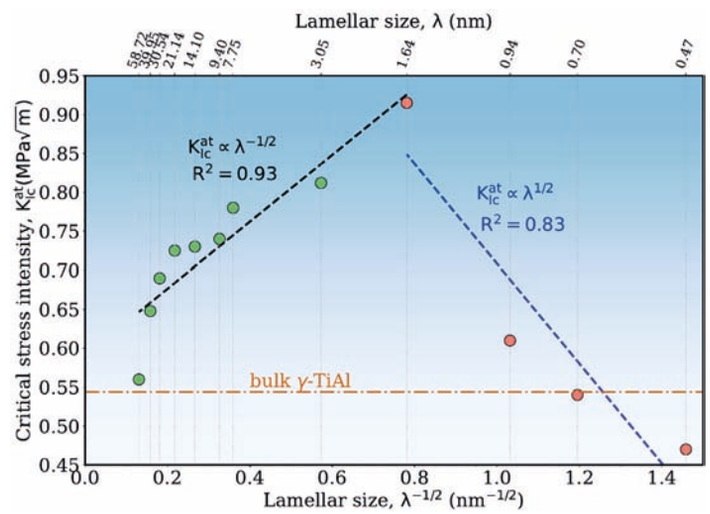


Fig. 6.6: Fracture initiation toughness K_{at}^{Ic} as a function of lamella spacing λ (upper abscissa), respectively $\lambda^{-1/2}$ (lower abscissa). For λ ≥ 1.64 nm a Hall-Petch type, and λ ≤ 1.64 $nm^{-1/2}$, an inverse Hall-Petch type behavior is observed. The bulk γ fracture initiation toughness is shown as the brown dashed line. Reprinted from [Neogi et al].

MMM

6.3. Data-Oriented Materials Modelling

Group leader:
Prof. Dr. Alexander Hartmaier

▸ 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. Worldwide, the activities in this direction have gained considerable momentum and span a wide range of applications now. Our research in this area focuses on two different activities: (i) the reconstruction of 3D microstructures from 2D surface maps, already highlighted above, and (ii) the implementation of trained machine learning algorithms to serve as constitutive models for plasticity and damage. In all these machine learning applications the physics-based models developed in our group are well-suited to produce the large amounts of data necessary to train machine learning algorithms to mimic real material behavior. 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.

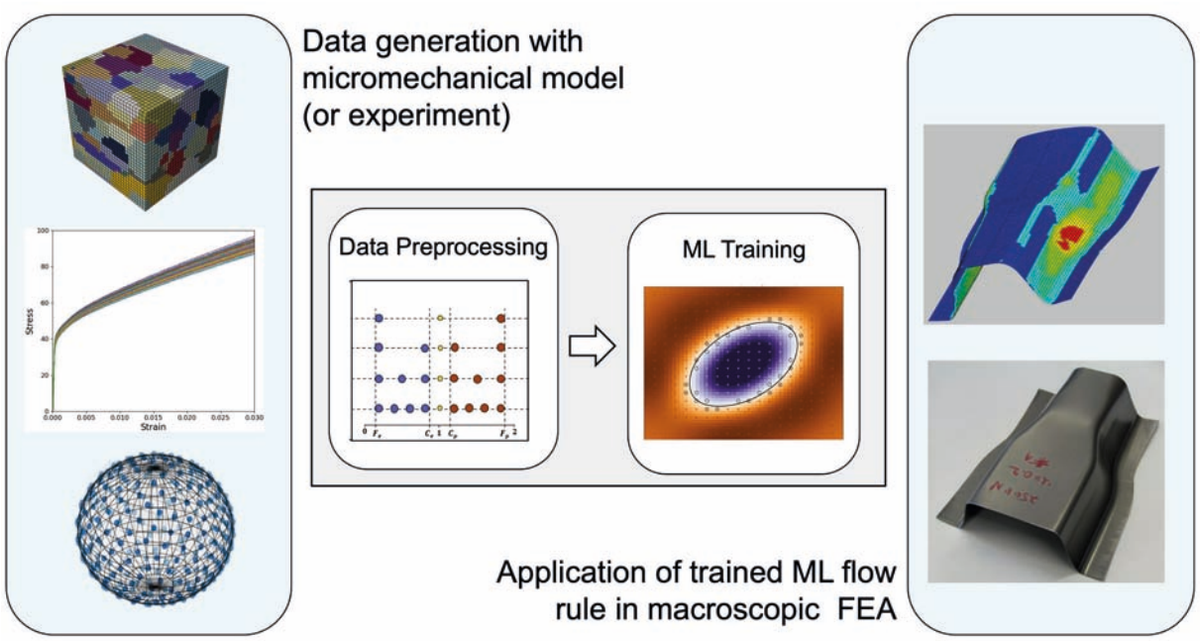


Fig. 6.7: Workflow to generate a Digital Material Twin from data gained with microstructure-sensitive models and to apply it in macroscopic simulations. (Open-Source code developed at ICAMS: https://github.com/ICAMS/pyLabFEA.git).

ICAMS

High-Performance Computing in Materials Science HPC

7. High-Performance Computing in Materials Science

Group leader:
Prof. Dr. Godehard Sutmann

Group members:
David Immel
Stephan Schulz

▸ Research

The research group High Performance Computing in Materials Science is working on the development of parallel methods and algorithms for the efficient simulation of materials science applications on different levels of approximation. Apart from original research, the group supports the development of simulation codes and efficient parallelization of programs, developed at ICAMS and international communities. Currently, one focus is given to new approaches of continuum mechanics modeling for plastic deformation, concurrent multi-level interaction potentials in atomistic simulations, 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 at Forschungszentrum Jülich and the CECAM community.

▸ Competences

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

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 the 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 improve sampling efficiency, the scheme is extended towards a biased MC approach, which takes into account the history of successful trial moves in the system. Parallelization of the hybrid MC/MS method is achieved by a Manager-Worker model which applies a speculative execution of trial moves which are asynchronously executed on the cores. The technique is applied to an Fe-C system including a dislocation as a symmetry-breaking perturbation in the system (*Fig. 7.1*)

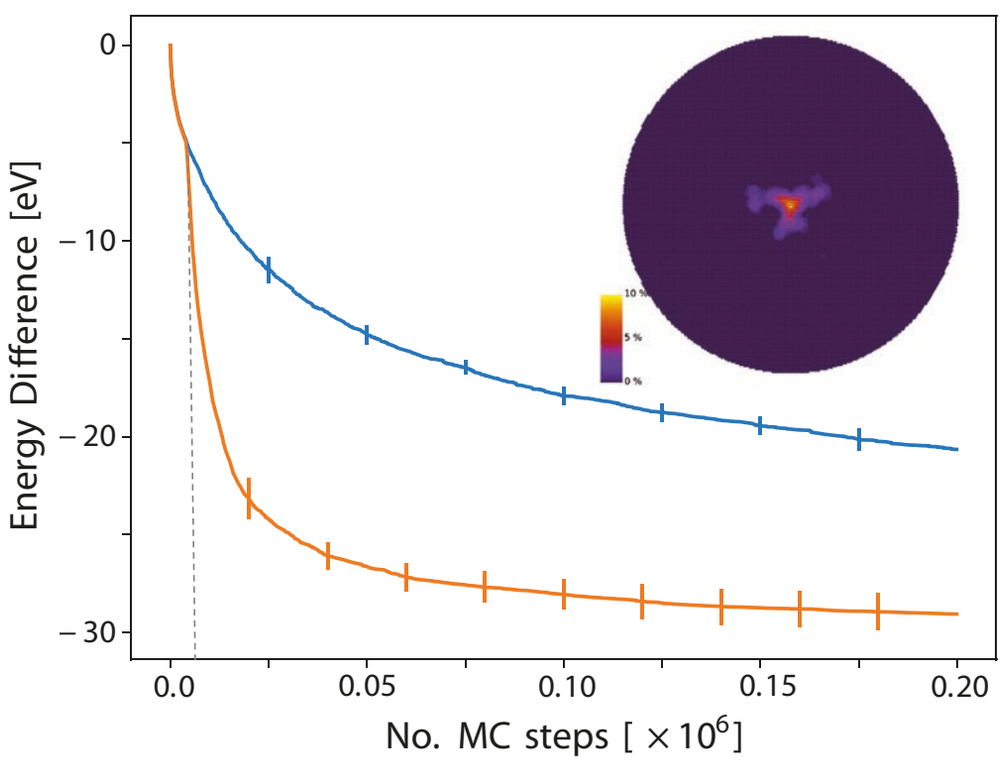


Fig. 7.1: Fig.1: Comparison between biased (orange) and unbiased (blue) Monte Carlo equilibration in terms of the configuration energy as a function of MC steps in the Fe-C system.

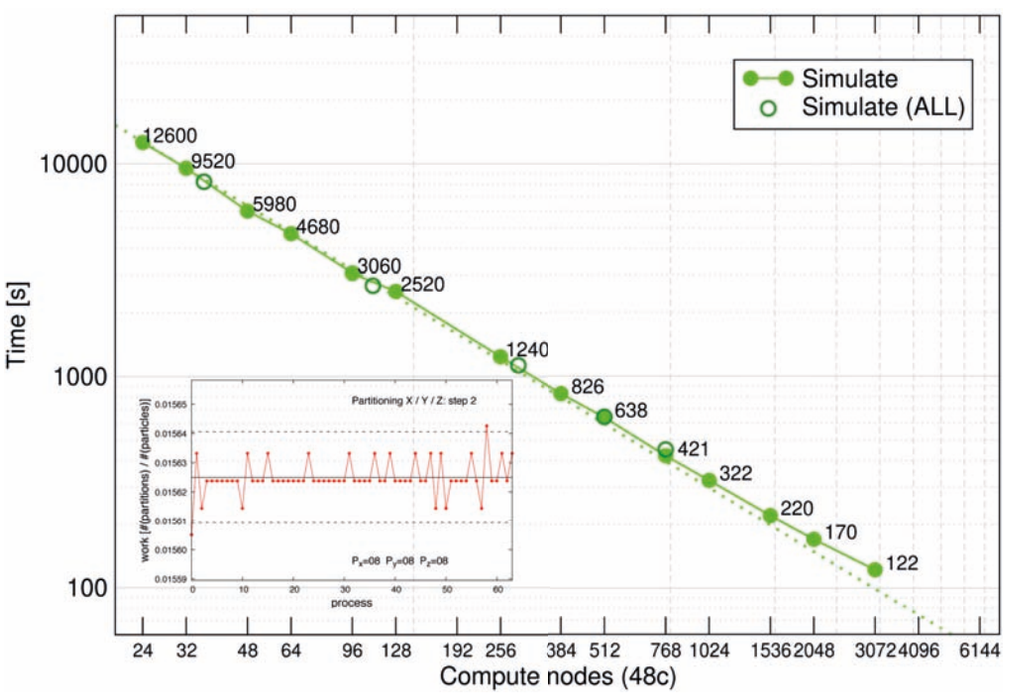
Kokkos-based implementation of MPCD on heterogeneous nodes

The Kokkos-based library Cabana, developed in the Co-design Center for Particle Applications (CoPA), is used for the implementation of Multi-Particle Collision Dynamics (MPCD), a particle-based description of hydrodynamic interactions. It allows a performance portable implementation, which has been used to study the interplay between CPU and GPU usage on a multi-node system. The program was tested on the Jülich syetm Juwels and at Los Alamos Crusher system. Both results show high consistency. As one result we see the most advantages in a homogeneous GPU usage since the data transfer as well as CPU/GPU usage are not balanced and lead to an unbalanced load distribution between the devices. To profit from the concurrent hybrid use of CPU/GPU devices, other types of domain decomposition, which allow a more balanced distribution, have to be considered in future, including unstructured decompositions, which allow for an arbitrary distribution of CPUs or GPUs along cartesian directions.

Load balancing for lattice Boltzmann blood flow simulations in HemeLB

The development of an efficient load-balancing method has been achieved for the simulation of a Lattice-Boltzmann method in the context of blood flow in a virtual human. This simulation includes lattices of more than 1010 lattice sites in a very inhomogeneous distribution. Progress has been made in enabling the HemeLB lattice Boltzmann code to simulate 3D macroscopic blood flow on a full human scale. Significant developments in load-balancing, based on histogram methods, allow a near-linear scaling performance of the code on hundreds of thousands of computer cores. (*Fig.7.2*)

Fig. 7.2: Wall clock time of a benchmark for the Lattice Boltzmann code HemeLB for a realistic blood flow simulation up to >140k cores. As an example, the inset shows the workload distribution on 64 cores with the load balancer ALL.



ICAMS

Scale-Bridging Simulation of Functional Composites SFC

8. Scale-Bridging Simulation of Functional Composites

Group leader:
Prof. Dr. Anna Grünebohm

Group members:
Aris Dimou
Lan-Tien Hsu
Susanne Kunzmann
Sheng-Han Teng

▸ Research

Ferroelectric perovskites (ABO3, or A'BX3 with A:alkali earth metals, A': Cs or molecules, B: transition metals and X: Cl,Br,I) are widely used in applications and promising for energy harvesting devices as well as for future efficient solid-state cooling devices based on the electrocaloric effect. All these applications share the following demands on materials design: Replace problematic elements and increase efficiency and reversibility in a broad and suitable operation range.

The group's goal is to design ferroelectric materials and composites with superior functional properties. Our approach is the scale-bridging optimization of microstructures and composite morphologies, combining the benefits of materials choice, controlled inhomogeneities, domain engineering and interface design. Our methods are scale-bridging simulations based on ab initio parametrization with high predictive power, which allow us to fundamentally understand and design the properties of materials systems.

▸ Competences

- Molecular dynamics and density functional theory simulations
- Ferroic materials and composites
- Functional (piezoelectric, dielectric, caloric, magnetic) responses
- Displacive phase transitions

One research focus in 2021/2022 was ferroelectric domain walls. We studied their thermal stability with atomistic and coarse-grained molecular dynamics simulations and cross-validated these methods. Particularly, we looked at the microscopic processes governing the domain wall dynamics driven by external electrical fields. We found that ultrafast-field pulses may drastically boost the domain wall velocity while inclusions may pin these. A second focus was on the impact of point defects, atomic ordering and concentration gradients on phase stability and ferroelectric switching in $BaTiO_3$ based solid solutions and composite materials.

Furthermore, a new project on displacive phase transitions in a broader material class has been recently started.

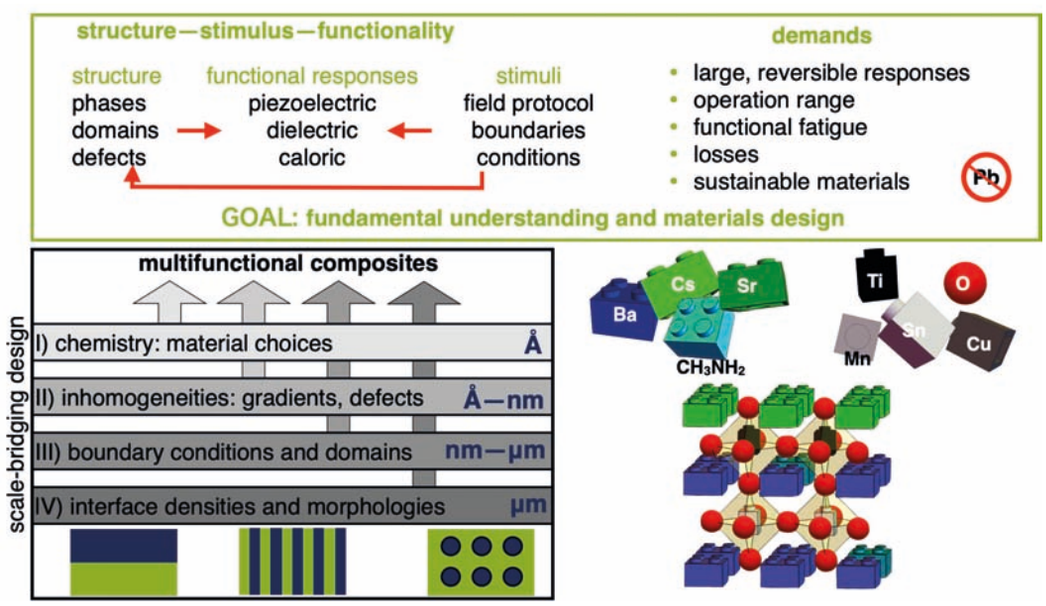


Fig. 8.1: Scale-bridging simulation of Functional Composites.

Domain wall acceleration by ultrafast field application

Optimizing ferroelectrics for contemporary high-frequency applications asks for ta fundamental understanding of ferroelectric switching and domain wall (DW) motion in ultrafast field pulses while the microscopic understanding of the latter is so far incomplete. To close this knowledge gap, ab initio-based molecular dynamics simulations are utilized to analyze the dynamics of 180° DWs in the prototypical ferroelectric material $BaTiO_3$. We discuss how ultrafast field application initially excites the dipoles in the system and how they relax to their steady state via transient negative capacitance. Excitingly, a giant boost of the DW velocity related to the nonequilibrium switching of local dipoles acting as nucleation centers for the wall movement is found. This boost may allow to tune the local ferroelectric switching rate by the shape of an applied field pulse.

R. Khachaturyan, A. Dimou, A. Grünebohm,
Domain wall acceleration by ultrafast field application: an ab initio-based molecular dynamics study,
Physica status solidi (RRL), 2200038, 2022

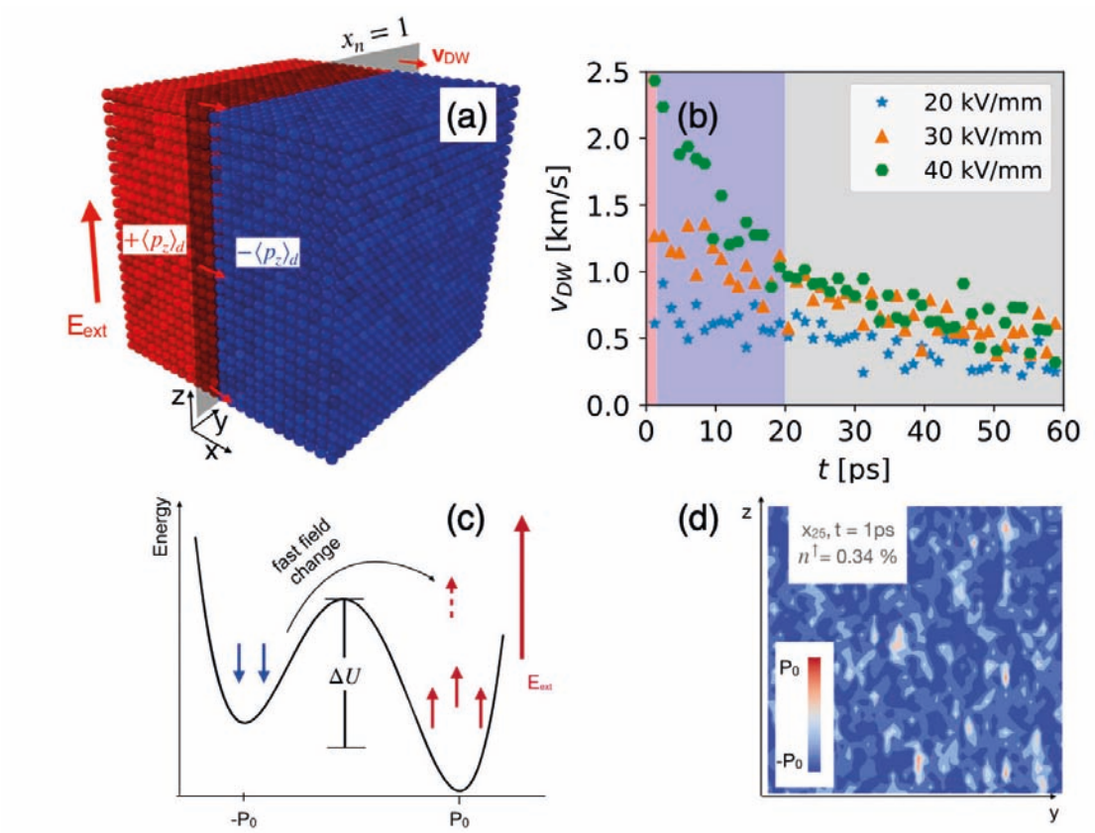


Fig. 8.2: (a) Atomistic model of a tetragonal 180° domain wall in $BaTiO_3$. Each sphere represents one unit cell and is color encoded by the polarization direction. (b) Field-induced velocity of domain walls for different field strengths. Excitingly, the ultra-fast application of the field initially boost the wall velocity. (c) Illustration of the underlying mechanism: Initially, the field aligns many local dipoles which are antiparallel to the surronding domain and act as nucleation centers for domain wall motion. The induced depolarization field results in a back relaxation of these dipoles and the wall slows down to its steady state. (d) Examplarly cut through the negative domain 0.1 ps after field application showing several small reversed clusters of dipoles.

Pinning of domain walls by strontium layer in $BaTiO_3$ perovskite

We use atomistic simulations to study the interactions between two-dimensional domain walls and Sr inclusions in the prototypical ferroelectric $BaTiO_3$. Based on nudged elastic band calculations we predict that the energy barrier for domain-wall movement increases in the vicinity of small planar Sr inclusions, which may act as pinning centers. We link this observation to the local increase in polarization by larger oxygen off-centering and validate our predictions by molecular dynamics simulations of field-driven domain walls at finite temperatures.

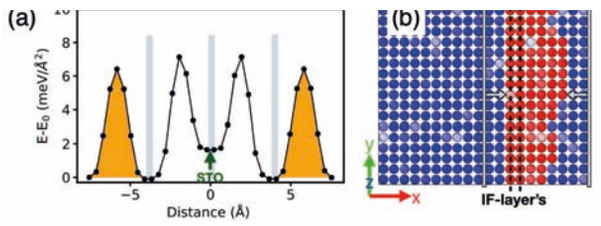


Fig. 8.3: (a) Change of the energy barrier for domain wall motion in $BaTiO_3$ at a $SrTiO_3$ inclusion as obtained by NEB simulations. (b) Pinning of a moving domain wall on a $SrTIO_3$ inclusion in Molecular dynamics simulations.

A. Dimou, P. Hirel, A. Grünebohm,
Pinning of domain walls by strontium layer in $BaTiO_3$ perovskite: an atomic-scale study, Physical Review B, 106, 094104, 2022

Thermal stability of nanoscale ferroelectric domains

Ultradense domain walls are increasingly important for many devices, but their microscopic properties are so far not fully understood. Here we use molecular dynamic simulations to study the domain wall stability in the prototypical ferroelectric $BaTiO_3$ combining core-shell pair potentials and a coarse-grained effective Hamiltonian. We transfer the discussion of the field-driven nucleation and motion of domain walls to thermally induced modifications of the wall without an external driving force. Our simulations show that domain wall dynamics and stability depend crucially on microscopic thermal fluctuations. Enhanced fluctuations at domain walls may result in the formation of critical nuclei for the permanent shift of the domain wall. If two domain walls are close – put in other words, when domains are small – thermal fluctuations can be sufficient to bring domain walls into contact and lead to the annihilation of small domains. This is even true well below the Curie temperature and when domain walls are initially as far apart as six unit cells. Such small domains are, thus, not stable and limit the maximum achievable domain wall density in nanoelectronic devices.

A. Klomp, R. Khachaturyan, T. Wallis, K. Albe, A. Grünebohm,
Thermal stability of nanoscale ferroelectric domains by molecular dynamics modeling, Physical Review Materials, 6, 104411, 2022

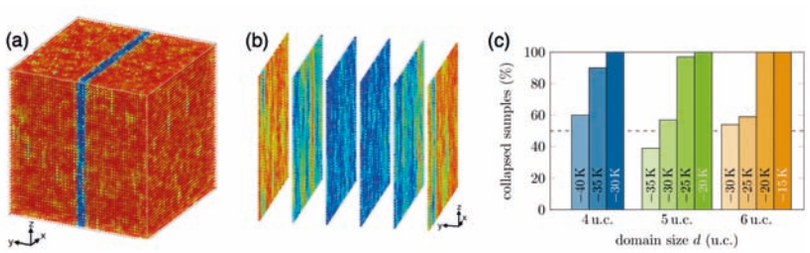


Fig. 8.4: Local polarization evolution and collapse of small ferroelectric domains from molecular dynamics simulation. (a) 3D representation of the full system; (b) Snapshot of the local polarization in an ultrathin domain (4 unit cells) before its collapse (c) Dependency of the fraction of samples that actually showed domain collapse during the first 200 ps on temperature and thickness.

ICAMS

Materials Informatics and Data Sciences MIDS

9. Materials Informatics and Data Sciences

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

Group members:
Dr. Ashish Chauniyal
Dr. Tushar Jogi
Benjamin Udofia
Lei Zhang

▸ Research

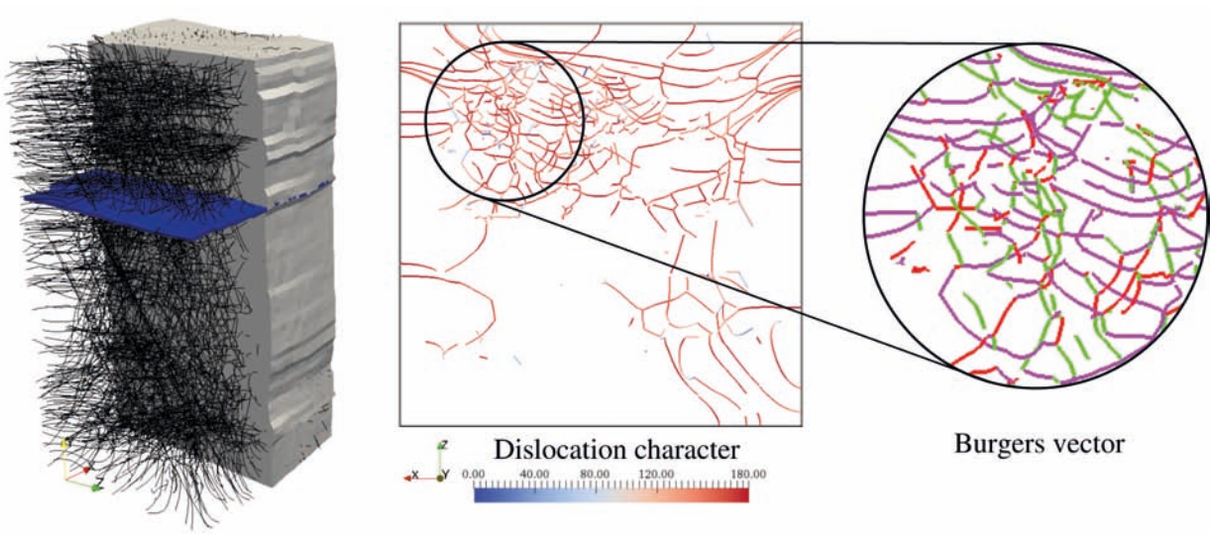
The activities in the group 'Materials Informatics and Data Science' in the two years since its instalment can be broadly categorized into the areas, dislocation-based plasticity modelling, and data fusion and knowledge extraction. Within the former area, we work on combining discrete dislocation dynamics coupling with the phase-field method, thus improving the experimental analysis of micromechanical experiments by tailored discrete dislocation simulations and contributions to the development of a library for the efficient computation of representations for atomic-scale learning, e.g. in the context of machine-learned interatomic potentials to improve the predictive capabilities of computational approaches. Within the latter, our current activities comprise data analysis to improve the characterization and synthesis of materials related to plasticity, electrochemistry, mechanochemical synthesis, high-throughput characterization, natural language processing, and knowledge graph development. Many of these activities are based on newly established collaborations within RUB and the UA Ruhr and serve as preliminary work for planned research in national and international collaborative projects. In particular, the interdisciplinary collaborations with colleagues from the faculty of Computer Science in overlapping topics show a huge potential for future joint research at the intersection of Materials and Computer Science.

▸ Competences

- Data fusion from experiments and simulations
- Materials data science and research data management
- Atomistic (Molecular statics and dynamics) and mesoscale (discrete dislocation dynamics) simulations of the mechanical behavior of materials
- Knowledge extraction and text mining

Data fusion torsion/experiment

Complex loading scenarios like torsion produce specific dislocation substructures, and analyzing these can help understand plasticity on the micron scale. Formation mechanisms are often only indirectly accessible in experiments due to a lack of resolution. Or it is just impossible to look into the sample during testing and obtain temporally resolved three-dimensional information of dislocations. The combination of experiments with tailored simulations provides insight into the formation mechanisms. But while experiments and simulations produce similar data, they are often not directly comparable. By combining results from small-scale experiments with discrete dislocation dynamics in the common language of "misorientations", we showed successful data fusion, and we explained dislocation structures and their behavior during torsion loading. This successful example shows that the key to fusing data is to find a common language between the two data sets. A new term for this common language in machine learning applications in materials science is 'descriptor'.



M. Stricker, M. Ziemann, M. Walter, S. M. Weygand, P. Gruber, D. Weygand,
Dislocation structure analysis in the strain gradient of torsion loading: a comparison between modelling and experiment,
Modelling and Simulation in Materials Science and Engineering, IOP Publishing, 30, 035007, 2022

Fig. 9.1: Dislocation structure of the <111> sample including a cross-section view containing a large surface step indicated by the blue plane. Only dislocations within the blue plane are shown. The indicated plane is a slice of height ≈66 nm. Dislocations arrange in hexagonal network patches of mostly screw orientations (center), each hexagon containing the three Burgers vectors of this plane (right, coloring according to Burgers vector).

Efficient implementation of atom-density representations

Atom-centered representations of molecular structures are critical to the success of modern atomistic machine learning. They form the basis for predicting properties of both materials and molecules, and for understanding and visualizing their chemical structures and compositions. Recently, it has been discovered that many of the most effective representations share a fundamental connection, which is a discretization of n-body correlation functions of the local atom density. This was the motivation for our contribution, the standardization and optimization of their evaluation. We presented an implementation called "librascal", which has a modular design that allows for developing refinements to the density-based formalism and for quickly prototyping new developments of rotationally equivariant atomistic representations. As an example, we discussed the Smooth Overlap of Atomic Position (SOAP) features, which is one of the widely used representations in this family, and showed how the expansion of the local density can be optimized for any choice of radial basis sets. We also discussed the representation within a kernel ridge regression model and analyzed how the computational effort scales for each step of the calculation. By applying data reduction techniques in feature space, we demonstrate how to reduce the total computational cost by a factor of up to 4 without impacting the model's symmetry properties and without significantly reducing its accuracy.

F. Musil, M. Veit, A. Goscinski, G. Fraux, M. J. Willatt, M. Stricker, T. Junge, M. Ceriotti,
Efficient implementation of atom-density representations,
The Journal of Chemical Physics, 154, 114109, 2021

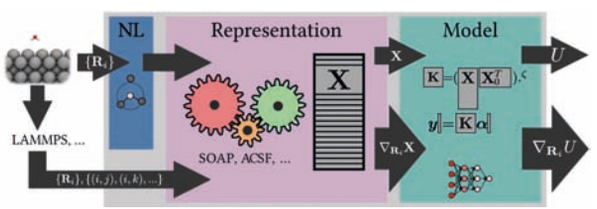


Fig. 9.2: Schematic depiction of the different components in librascal for the evaluation of atomic energies and forces for atomic-scale machine-learning models.

First steps towards Materials Knowledge Graphs

Within the Collaborative Research Centre Transregio 103 "From atoms to turbine blades – a scientific basis for a new generation of single-crystal superalloys" we started to develop the first tools to extract and reuse scientific knowledge communicated in text form. For one article (Scholz et al, Materials, 2021, 14), we created a specific ontology to represent the information contained. This information includes sample preparation methods, treatment processes, and characterization methods. We then combined the data model (ontology) with the data of the article to create a knowledge graph of this paper. Next steps include the development and deployment of tools from the field of natural language processing and image recognition to automate this process to make available the vast amount of knowledge contained in millions of already-published papers.

S. Baghaee Ravari, M. Stricker,
A knowledge graph for superalloys – one step in the digitalization process of knowledge,
Materials Research Department Newsletter, 15, 2022

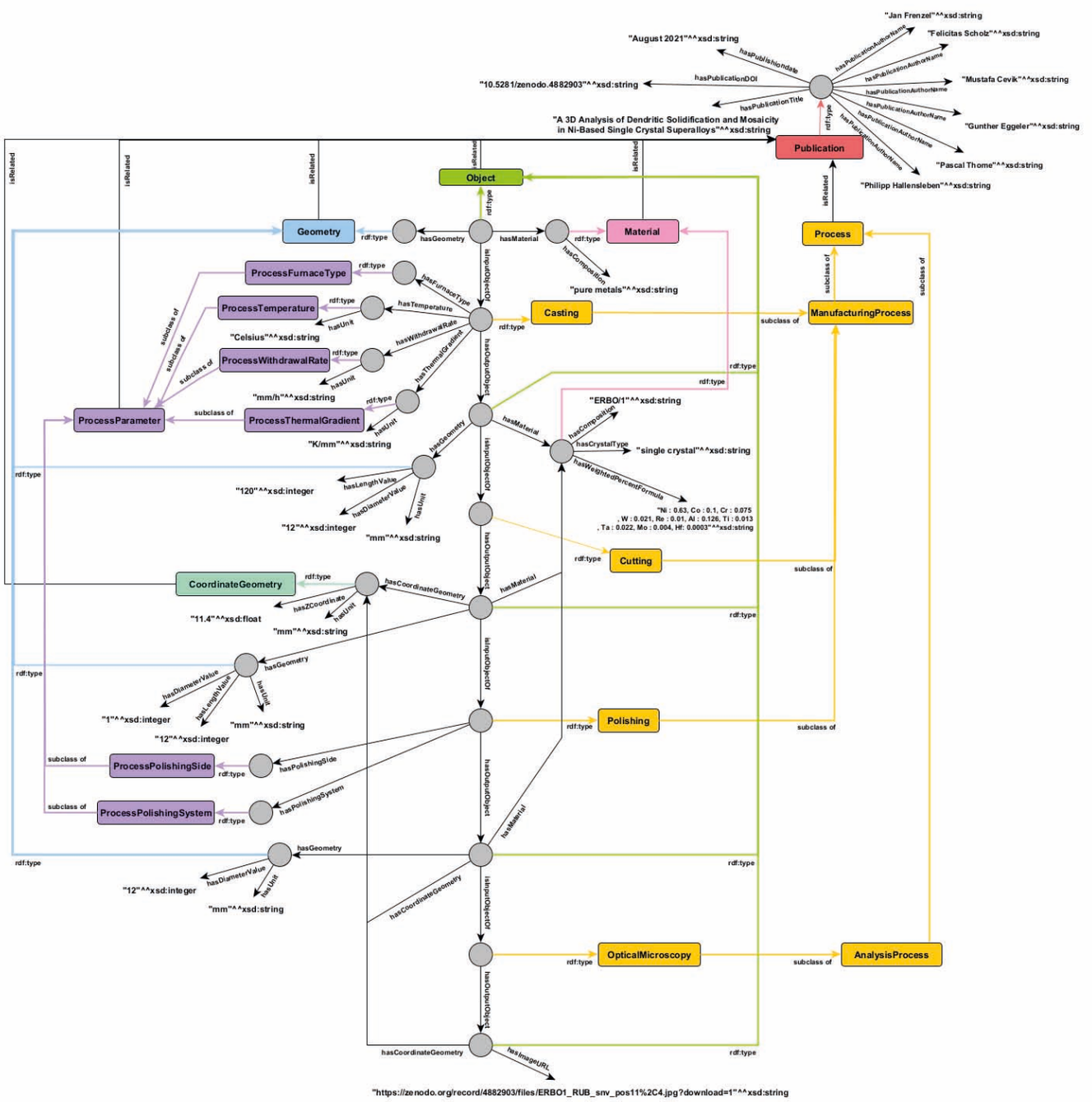


Fig. 9.3: Knowledge graph for a paper presenting a 3D analysis of dendritic solidification and mosaicity in Ni-based single crystal superalloys.

ICAMS

Advanced Study Group Ab Initio-Based Modelling

10. Advanced Study Group Ab Initio-Based Modelling

Prof. Dr. Jörg Neugebauer
Dr. Tilmann Hickel

▸ Research

The Advanced Study Group (ASG) Ab Initio-Based Modelling serves as a centre of competence for different concepts in materials modelling in order to support the research at ICAMS, in particular on the electronic scale. It develops, implements, and applies ab initio-guided computational methodologies and toolsets that allow for an accurate prediction of properties of advanced structural and functional materials in realistic environments.

Being mainly located in the department of Computational Materials Design at the Max-Planck-Institut für Eisenforschung in Düsseldorf, the atomic-based mechanisms that determine the microstructure in structural and functional materials form a central part of the contribution to ICAMS. In many cases, these mechanisms are connected with thermodynamic considerations. The example in (*Fig. 10.1)* shows how large regions of chemical compositions are considered in order to analyze precipitations in steels – in this case, carbides – their stability and hydrogen solubility. In this way, multiple physical properties are considered in combined materials models. In the last years, the ASG has extended their computational tools to describe the sophisticated interplay of chemical, magnetic and structural degrees of freedom to defects. The example in (*Fig. 10.2*)shows the dependence of the segregation of Mn atoms to grain boundaries on the magnetic ordering. The strong effects give rise to defect phase transformations, a phenomenon that is currently systematically investigated within the ASG.

Since the underlying highly accurate and computationally efficient methods require complex simulation protocols, the ASG developed over the last years pyiron – a platform that provides an integrated development environment to implement, test and employ computational tools such as empirical potentials of multicomponent alloys (*Fig. 10.3*). It does not only provide the user with a standardized interface for the communication between different codes and routine but also allows easy upscaling to high-throughput studies. As a result, the time needed to become acquainted with new tools is dramatically reduced, productivity is boosted and the exchange with external partners and, in particular, ICAMS is supported. Consequently, these concepts form a core component of large-scale initiatives like Plattform MaterialDigital and the National Research Data Infrastructure for Materials Science & Engineering (NFDI-MatWerk).

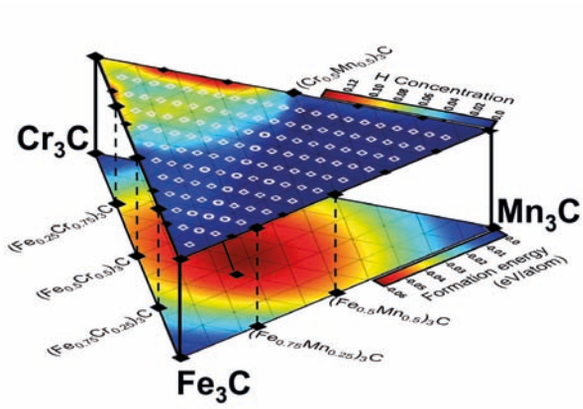


Fig. 10.1: Ab initio-based investigation of high-entropy carbides as a function of composition; the lower plane shows their thermodynamic stability at 650 K. The upper plan shows how much hydrogen these carbides can absorb from the environment. In this way, the structural and functional properties of these materials can be correlated.

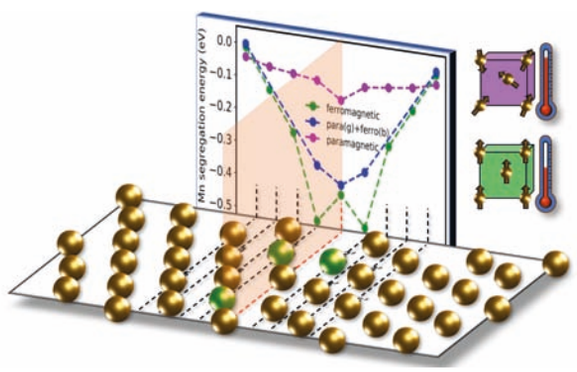


Fig. 10.2: Within the ASG, advanced ab initio-based thermodynamic methods are used to predict the thermodynamics of defect phase stability in multi-component alloys. The diagram shows the segregation energies of Mn atoms (green spheres) to the Σ5(310) grain boundary with dashed lines indicating layers next to the GB layer (red line). The behaviour in the ferromagnetic and the paramagnetic states are compared.

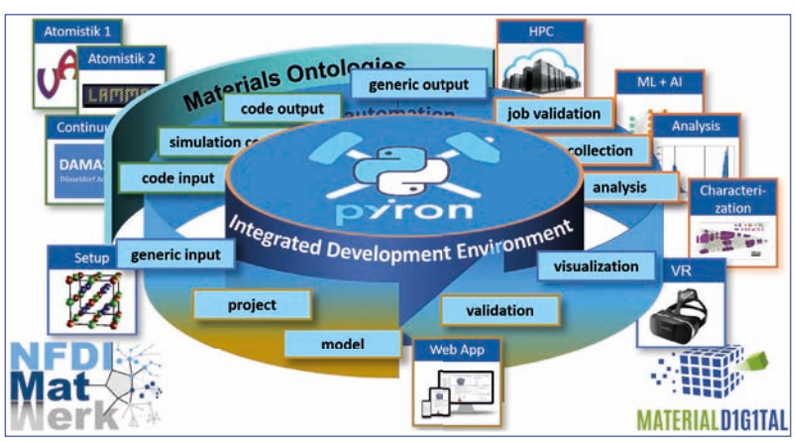


Fig. 10.3: By using the integrated development environment pyiron, generic workflows for complex simulation protocols can be executed and a large set of tools become accessible, while the technicalities of the interfaces are shielded from the user.

ICAMS

Advanced Study Group Input Data and Validation

11. Advanced Study Group Input Data and Validation

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

The Advanced Study Group (ASG) "Input Data and Validation" provides strong experimental expertise in ICAMS. We investigate elemental processes of microstructure evolution and related effects on the properties of structural and functional engineering materials. We interact with other ICAMS groups and provide experimental data for joint research activities, for example through the collaborative research center SFB/TR 103 ("From atoms to turbine blades"). The group also has a strong teaching commitment within the new Bachelor program "Materialwissenschaft" (MaWi, materials science), which started in the winter semester 2021: Gunther Eggeler and Jan Frenzel provide various lectures, e.g. "Experimental Methods in Materials Science", and a laboratory course introducing MaWi students to experimental aspects of materials science and providing them with first hands-on expertise in materials processing and microstructural characterization. They learn how as-cast microstructures of aluminium alloys can be modified by thermomechanical treatments and how optical and scanning electron microscopy can be combined to retrieve microstructural information related to different length scales. *Figure 1.11* shows how Felicitas Werner and Aron Trappmann prepare chocolate ice cream for a small group of MaWi students by using liquid nitrogen. This small demonstration was part of a lecture unit on experiments at low/cryogenic temperatures.

Fig. 11.1: Example for teaching in the new Bachelor program "Materialwissenschaft" (MaWi). Felicitas Werner and Aron Trappmann demonstrate the application of liquid nitrogen to a group of bachelor students.

In the following sections, we present research examples from different fields. In the first one, we consider an SFB/TR 103 project, which addresses the formation of low-angle misorientation defects during dendritic solidification of single crystal Nickel-based superalloys. Superalloys are key materials in highly efficient gas turbines, representing important backup systems for renewable energy sources. Our research activities are conducted in the frame of the collaborative research center SFB/TR 103, which is in its final funding phase. During the last years, a novel tomographic characterization approach has been established by Felicitas Scholz, a prior member of our group. After her graduation, Felicitas Scholz worked as a science manager in the Materials Research Department (MRD) at RUB prior to receiving a Feodor Lynen Fellowship for a research visit at the Institut de Recherche de Chimie Paris (Chimie ParisTech – PSL). Recently, our tomographic characterization technique, which was developed to analyze the growth behavior of dendrites, has been significantly improved by data science approaches. Pascal Thome and Alexander Richter have developed new machine-learning procedures that are able to identify and reconstruct superalloy dendrites by using tomographic 2D image data as input. In a first step, optical micrographs of as-cast superalloys are generated by an optimized metallographic procedure. Afterwards, neuronal network-based techniques are applied to scan the image data to detect and evaluate the growth trajectories of a large number of individual dendrites. This approach not only allows tracing the evolution of microstructures across various length scales (from the micrometer to the centimeter scale). It can also be used to monitor rare events like dendrite deformation processes, and it can reveal relationships between dendrite groups. *Figure 2.11* presents an example of how our tomographic analysis is applied to reconstruct the growth behavior of dendrites (*Figure 11.2a-c*). *Figure 2.11d* shows an example where several generations of dendrites have evolved from one single parent dendrite (lower part of *Figure 11.2d*) during Bridgman solidification (growth direction: from lower towards upper image part).

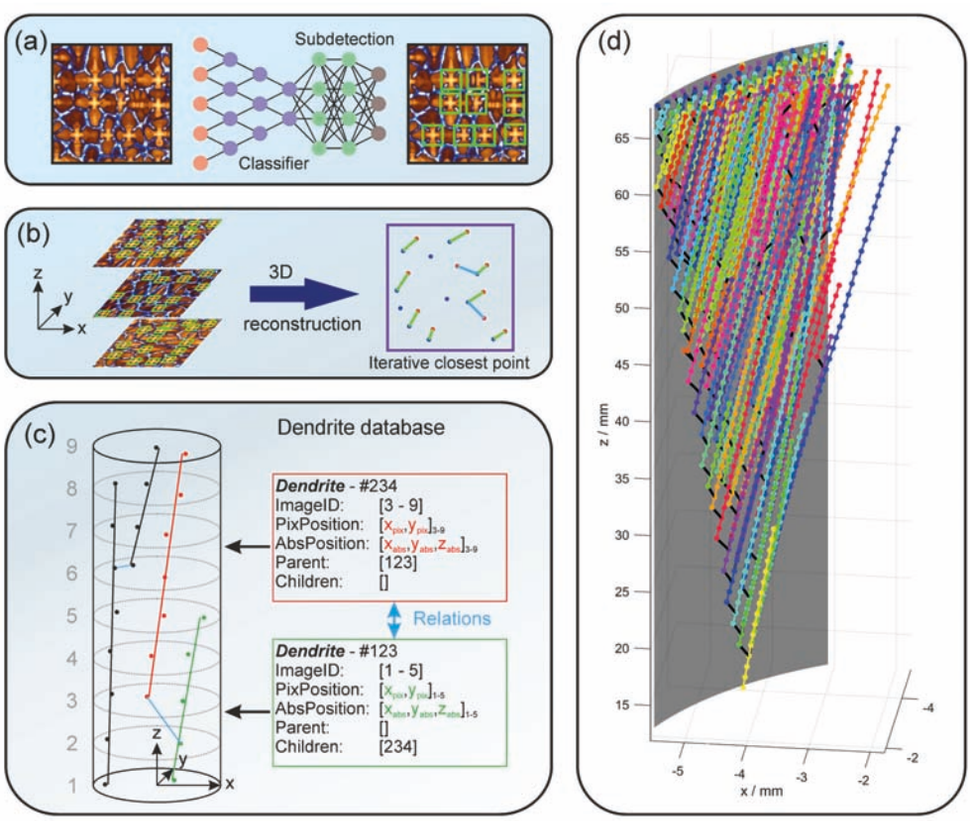


Fig. 11.2: Neuronal network-based 3D-analysis of dendrite growth phenomena. (a-c) Reconstruction of dendrites from tomographic image data, (d) example of how dendrite branching promotes the evolution of new dendrite populations which emanate from one yellow dendrite (bottom of Figure 2d).

As a second research example, we consider sustainable metallurgy of NiTi shape memory alloys. This research effort is conducted in the framework of the new International Max Planck Research School for Sustainable Metallurgy (IMPRS SusMet). Shape memory alloys represent a class of functional materials which show the fascinating ability to re-establish a pre-programmed geometry after a large deformation exceeding conventional elastic strain limits. The shape memory effect is based on a reversible martensitic transformation. Research on shape memory alloys, which started with Prof. Erhard Hornbogen in Bochum, has a long tradition at the Institute for Materials. Recently, after Bochum became one of the important places where this type of material is produced by our spin-off company Ingpuls, questions related to recycling and sustainable ingot metallurgy of Nickel-Titanium shape memory alloys became relevant. Recycling of NiTi is highly attractive since the production of pure raw materials, Nickel and Titanium, is associated with high energy input and the generation of large amounts of CO_2 emissions. However, recycling NiTi is by no means easy as this material has low tolerances for impurities, especially for oxygen and carbon. In our project, Sakia Noorzayee studies how repeated laboratory scale recycling cycles affect microstructures, martensitic transformations and thus shape memory properties. In this work, different processing strategies are considered which aim at keeping impurity concentrations at low levels. We also investigate whether it is possible to establish "second-life applications". For example, shape memory alloys with high transformation temperatures, which initially were applied as actuators, could obtain a second life as pseudoelastic materials, after their transformation temperatures decreased by unavoidable concentration changes during recycling. *Figure 11.3* present aspects of NiTi ingot metallurgy. NiTi alloys are usually prepared in graphite crucibles, *Figure 11.3a*. During processing and especially recycling, they can pick up certain amounts of impurities providing to the formation of brittle phases *Figure 11.3b*.

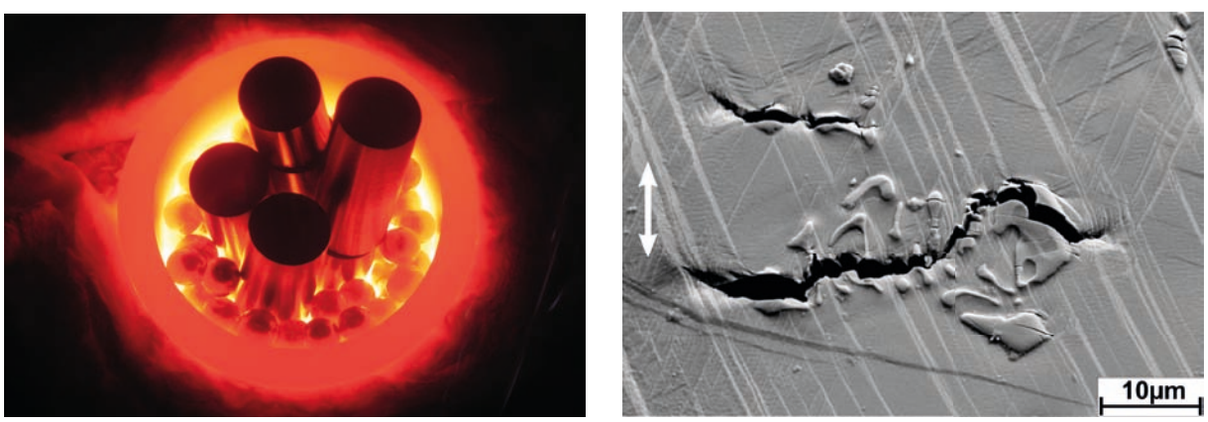


Fig. 11.3: Sustainable ingot metallurgical preparation of NiTi and impurity-related secondary phases. (a) melting of Nickel and Titanium in a graphite crucible. (b) SEM in-situ experiment, which demonstrates the risk of crack formation and fracture. During mechanical loading (white arrow: loading direction), small cracks emanate from oxygen-rich phases.

ICAMS

Advanced Study Group Processing and Characterisation

12. Advanced Study Group Processing and Characterisation

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

▸ Research

The ASG Processing and Characterisation, located at the Steel Institute (Institut für Eisenhüttenkunde – IEHK) at RWTH Aachen University, focuses on the major topics materials characterisation, advanced computer simulation of materials, materials processing, and damage mechanics. Our ultimate aim is to understand the mechanisms behind the physical, mechanical, and microstructural properties of steels and other advanced engineering alloys, to be able to improve their macroscopic behaviour through transformations and variations of the microscopic phases, and to design advanced solutions for alloy production, processing and application. The scientific approach of the institute is to use a combination of different mechanical and physical testing methods with advanced numerical approaches in order to investigate the bulk properties of different metals and alloys at sub-zero temperatures as well as room and elevated temperatures.

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

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

In a recently completed AiF-EFB project, we applied the integrated computational materials engineering (ICME) approach (*Fig. 12.1a*), which uses a thermo-micro-mechanical (TMM) damage model, capable of predicting strain hardening and damage behavior of metallic materials based on the microstructure evolution during deformation. The macroscopic body is discretized into multiple material points (*Fig. 12.1b*), each of which corresponds to a representative material volume (RVM). Microstructural features such as dislocations and voids were selected for this work. The distribution of microstructural features (dislocation density and void fraction) in an RVM were averaged into a single state variable (based on type), also known as microstructural state variable (MSV). Evolution equations for these MSVs were defined based on the associated physical phenomena.

As a result of plastic deformation, the MSV evolves and indicates the current state of the material's microstructure. This information is used in the calculations of macroscopic responses such as stress. Based on the type of loading and the amount of plastic deformation, the damage might accumulate in the material, and as a

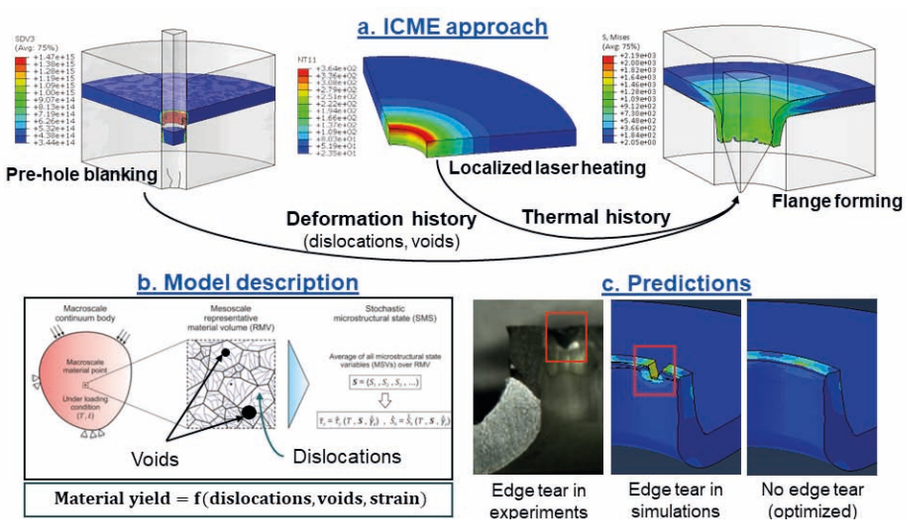


Fig. 12.1: a. process chain simulations using an ICME approach; b. TMM material model definition; c. experimental outcomes and predictions made using TMM simulations.

result, it fails. The only input required for the model is the initial state of the material (initial values of MSVs). When used in the simulation of a multi-step process chain the evolved MSVs at the end of the previous step are transferred as the initial condition of the next step to transfer the deformation history from one process to the other.

In this work, we developed a laser-assisted hole-flanging process chain. The process chain had three steps – pre-hole blanking, localized laser heating, and flange forming. The goal was to optimize the process to yield defect-free flanges. Most of the optimization was done using simulations with the TMM model to reduce experimental effort. To enhance the reliability of the prediction, the deformation history from the pre-hole blanking process (final MSVs – dislocation density and void fraction) and the thermal history (final temperature distribution) resulting from localized laser heating were transferred as an initial state to final flange forming simulations. This ICME approach provides more reliable predictions, as evidenced by the high agreement with experimental results (*Fig. 12.1c*).

Another activity of the ASG was the development of the web application idCarl (intelligent digital Computational advanced research laboratory) as a comprehensive research data management (RDM) system (*Fig. 12.2*). IdCarl is designed to describe and manage experimental data based on a material description ontology.

In contrast to existing RDM solutions, idCarl supports the creation and adjustment of processing chains, e.g. thermomechanical treatments, microstructure analysis and mechanical testing of engineering materials. The experimental data related to these materials is automatically connected to the designated process step with a unique material ID and is finally represented with a user-friendly chart view so that the specific material properties can be monitored along the selected processing chain. For all design considerations in the tool development, the ASG followed FAIR (Findability, Accessibility, Interoperability, and Reusability) principles as a major requirement for the practical use of RDM software. Together with ICAMS and IWM Freiburg, the ASG collaborates in "iBain", a project within BMBF's Material Digital platform, with the goal of developing an intelligent workflow to predict fatigue properties of bainitic steels. In this project, idCarl allowed building a material database for sharing machine-readable data (connected to associated processes by material-IDs) among all project partners.

Furthermore, with the modular design of the web application, the functionality can be expanded by integrating other material analyses or simulation tools and/or applications. So far, modules are available to automatize the analysis of tensile test data, electron microscopy images of bainite, and optical emission spectroscopy (OES) data. These modules and idCarl are containerized using docker for straightforward sharing with the scientific community.

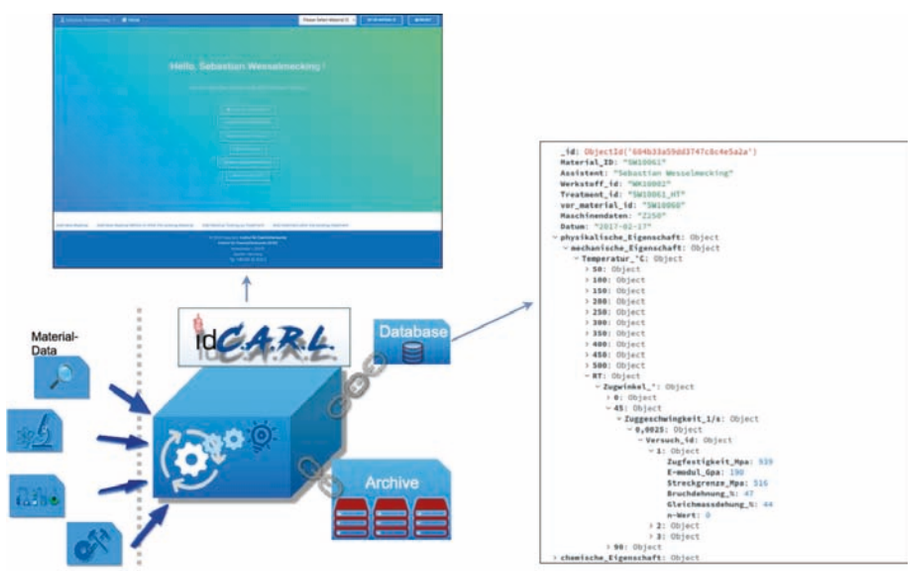


Fig. 12.2: Schematic representation of idCarl as data transformer: Processing of material data from experiments.

IC AMS

Advanced Study Group Diffusion and Microstructure Analysis

13. Advanced Study Group Diffusion and Microstructure Analysis

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

▸ Research

The ASG employs a range of complementing experimental methods to analyze the underlying physical mechanisms and microstructural origins of macroscopic materials behavior.

Specific emphasis is on the coupled analysis of
- atomic transport,
- atomic-level structure
- thermodynamic properties

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

Selected highlights from the studies as ASG in 2021-2022:

Decelerated aging in metallic glasses by low-temperature thermal cycling
(together with Prof. F. Varnik)

Differential scanning calorimetry measurements on different bulk metallic glasses show no measurable rejuvenation upon deeply cooled (cryogenic) thermal cycling, (*Fig. 13.1*). This applies both to as-quenched and well-annealed samples. Extensive molecular dynamics simulations of a generic model glass former corroborate these observations. We disentangle the effects of aging from those of thermal treatment and show that aging is slowed down but not stopped – neither reversed – during thermal cycling. These observations are corroborated further by a survey of energy distribution, which continues narrowing, albeit with a smaller rate, (*Fig. 13.2*).

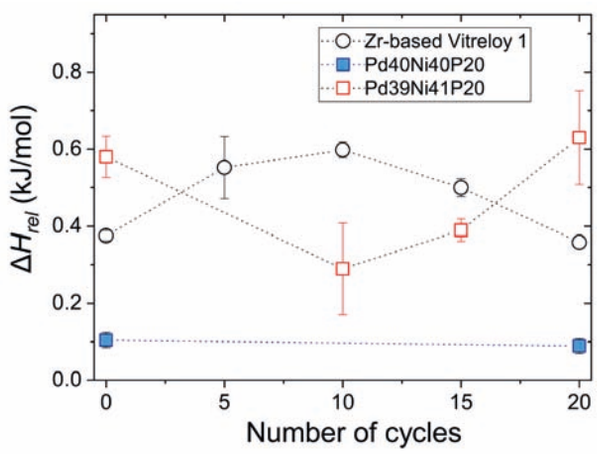


Fig. 13.1: Heat of relaxation as a function of the number of thermocycles for PdNiP (two compositions, squares) and Zr-based Vitreloy 1 (circles) glasses.

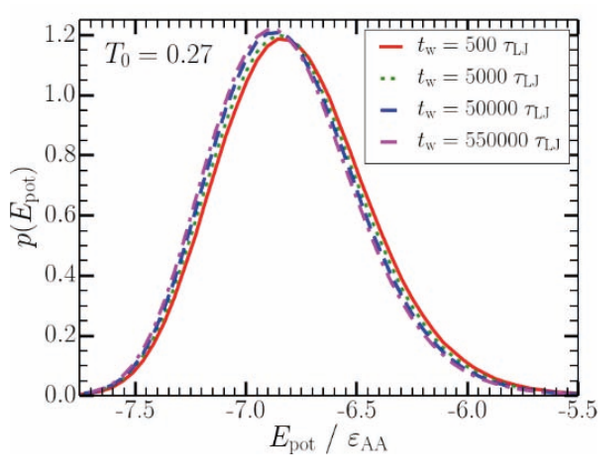


Fig. 13.2: Distribution of potential energy per particle for B-atoms evaluated after different aging times t_w. A narrowing of the distribution is seen as well as a shift of the mean energy level towards lower potential energy values.

M. Bruns, M. Hassani, F. Varnik, A. Hassanpour, S. Divinski, G. Wilde, Decelerated aging in metallic glasses by low temperature thermal cycling, Physical Review Research 3, 013234, 2021.
doi: 10.1103/PhysRevResearch.3.013234

Model for non-equilibrium vacancy diffusion applied to study the Kirkendall effect in high-entropy alloys
(together with Prof. I. Steinbach)

Impact of non-equilibrium vacancy concentration on the Kirkendall porosity formation is studied in the framework of a developed model of the multi-component diffusion with vacancies, which includes the intrinsic fluxes with vacancy gradient and non-ideal sources and sinks for vacancies. Interaction parameters between the components and vacancies are introduced, which have strong effects on the equilibrium vacancy concentration in alloys and on thermodynamic factors. The diffusion profiles of components and vacancies are simulated and a good agreement is obvious, (*Fig. 13.3*). The different intensities of the vacancy annihilation/generation and different initial vacancy distributions were considered, (*Fig. 13.4*). The numerical results demonstrate that the diffusion profiles of substitutional components slightly depend on the sink/source intensity if the none-zero net flux of substitutional components is not significant and the sources and sinks of vacancies are not sparse, whereas the porosity depends very strongly and correlates with the vacancy distribution. For the simulation of variable equilibrium vacancy concentrations using the MDV, the corresponding interaction parameters related to vacancies are necessary to be included in the thermodynamic assessment.

C.-H. Xia, J. Kundin, I. Steinbach, S. Divinski, Model for non-equilibrium vacancy diffusion applied to study the Kirkendall effect in high-entropy alloys, Acta Materialia 232, 117966, 2022.
doi: https://doi.org/10.1016/j.actamat.2022.117966

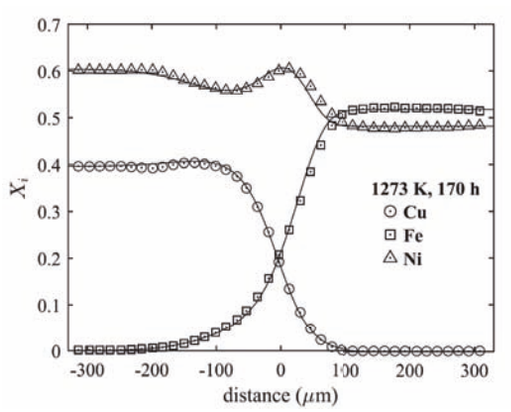


Fig. 13.3: Experimental (symbols) and calculated (lines) composition profiles for the Cu-60.4Ni/Fe-48.2Ni couple annealed at 1273 K for 170 h.

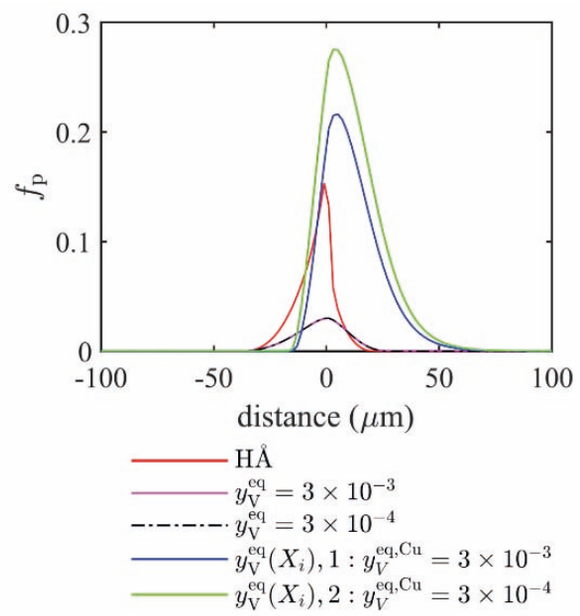


Fig. 13.4: Impact of vacancy production and interaction parameters on the predicted maximum pore fraction..

Advances in Understanding Diffusion in Multi-Principal Element Systems
(together with Prof. I. Steinbach)

Recent advances in the field of diffusion in multi-principal element systems are critically reviewed, with an emphasis on experimental as well as theoretical approaches to determining atomic mobilities (tracer diffusion coefficients) in chemically complex multicomponent systems. The brand-new results are shown in (*Fig. 13.5*) for FCC, BCC and HCP high-entropy alloys. The newly elaborated and augmented pseudo-binary and pseudo-ternary methods are shown to provide a rigorous framework to access tracer, intrinsic, and interdiffusion coefficients in alloys with an arbitrary number of components. Utilization of the novel tracer-interdiffusion couple method allows for a high-throughput determination of composition-dependent tracer diffusion coefficients. A combination of these approaches provides a unique experimental toolbox to access diffusivities of elements that do not have suitable tracers. The pair-exchange diffusion model, which gives a consistent definition of diffusion matrices without specifying a reference element, is highlighted.

A. Dash, A. Paul, S. Sen, S. Divinski, J. Kundin, I. Steinbach, B. Grabowski, X. Zhang, Recent advances in understanding diffusion in multi-principal element systems, Annual Review of Materials Research 52, 383-409, 2022.
https://doi.org/10.1146/annurev-matsci-081720-092213

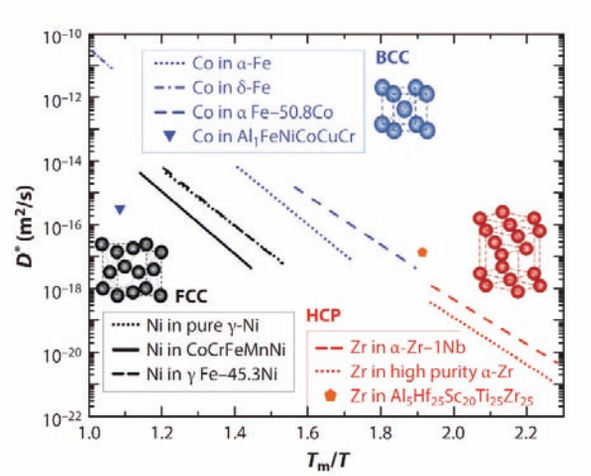


Fig. 13.5: Tracer diffusion coefficients, D, of selected constituting elements in FCC (Ni, black lines), BCC (Co, blue lines), and HCP (Zr, red lines) systems as the function of the inverse homologous temperature, T_m/T. The corresponding diffusion rates are compared for pure elements [Ni, α- and δ-Fe, and α-Zr], binary alloys [γ-Fe–Ni, α-Fe–Co, and α-Zr–Nb] and high-entropy alloys [CoCrFeMnNi, $Al_1FeNiCoCuCr$, and $Al_5Hf_{25}Sc_{20}Ti_{25}Zr_{25}$]. T_m is the melting point of the corresponding compounds.*

ICAMS

Advanced Study Group Continuum Mechanics

14. Advanced Study Group Continuum Mechanics

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

▸ Research

Simulation of crack propagation through metal matrix microstructures

To increase the wear resistance of cutting and drilling tools, one often applies reinforcement layers made of metal matrix composites, which consist of a ductile metallic matrix with embedded, brittle ceramic inclusions. One dominant wear mechanism is surface spalling, where subcritical crack propagation through the material's microstructure governs the macroscopic wear. [Wingender and Balzani 2022] present a novel, efficient method for the simulation of crack propagation through microstructures, which are given as voxel data. The method considers an extended eigenerosion approach to capture brittle and ductile fracture at finite strains, which appear at the microscale. Therein, the crack is numerically described by finite elements, which are iteratively eroded whenever a generalized Griffith criterion for brittle and ductile fracture is fulfilled. In order to enable mesh-independent simulations, a non-local normalization of the crack surface entering the fracture criterion is considered. Major advantage of such an eigenerosion approach over competitive approaches like phase field fracture is that it does not require any additional primary variables. Since three-dimensional data on microstructures is usually available as voxel data, a novel method is proposed, which particularly adapts the eigenerosion approach to this kind of data set. To this end, an extended finite cell method is considered, where an optimal set of subcells is constructed. To connect this with the eigenerosion approach, an algorithm is formulated, where the finite subcells are switched to refined finite elements whenever the crack enters a finite element. Thereby, an automated adaptive mesh refinement at the crack tip is obtained while still allowing for an efficient representation of material interfaces where no crack appears. Note that this mesh refinement does not require any additional projection of history variables as the integration of the refined elements matches the previously considered finite subcells. The performance of the proposed method has been shown by several numerical examples including the calculation of crack propagation through idealized and real metal matrix composites, cf. *Fig. 14.1*. The method can also be considered advantageous for the simulation of microcracks in other materials such as metamaterials using direct micro-macro-transition approaches as proposed in [Tamsen and Balzani 2021].

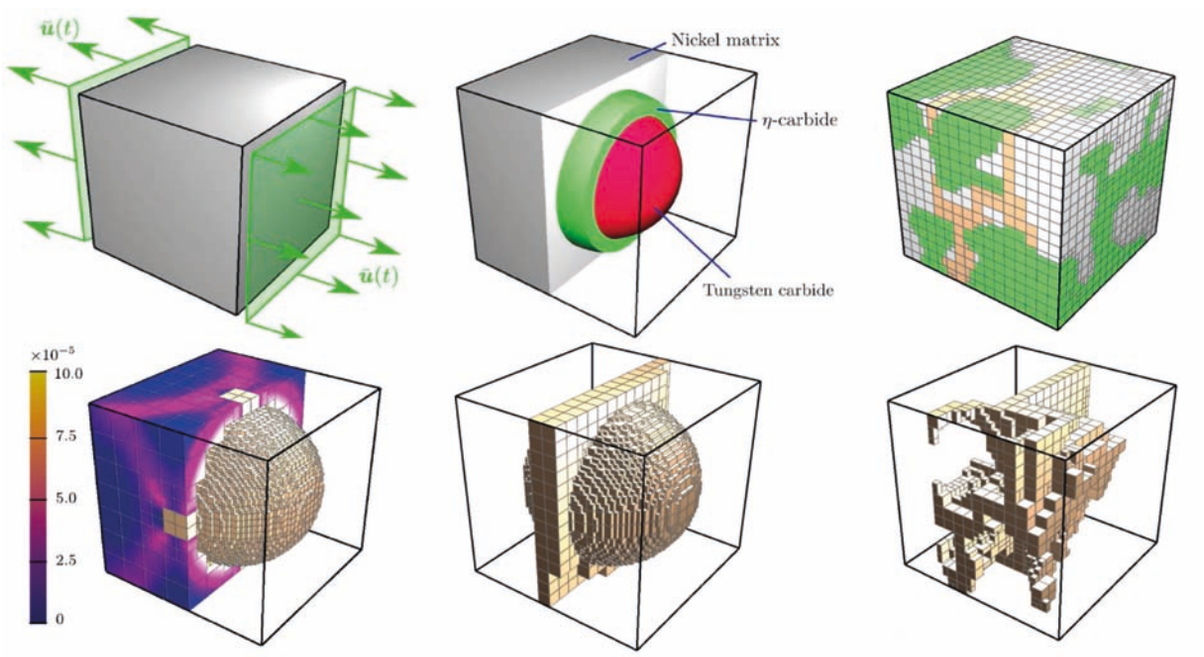


Fig. 14.1: Simulation of crack propagation in a three-layer benchmark problem (left four pictures) and in a real microstructure of a metal matrix composite obtained from Micro-CT (right two pictures). The cracks are depicted in gold and form a quite sophisticated, branched shape mainly going around the inclusions.

Enhanced model-free data-driven computational mechanics

The Advanced Study Group 'Continuum Mechanics' activities involve research on model-free data-driven computational mechanics devised to overcome the necessity of traditional material modeling in mechanics. Kerem Ciftci and Klaus Hackl perform this research at the Institute of Mechanics of Materials at Ruhr-University Bochum. We replace the associated phenomenological constitutive models with numerical simulations based on data sets of representative samples in stress-strain space. The method is based on the nearest-neighbors approach. Precisely, in continuum mechanics, the optimization problem consists of computing the closest point in the data set consistent with the compatibility and equilibrium condition of the problem. Thus, the data-driven scheme bypasses the empirical material modeling step, providing an alternative formulation of the classical boundary-value problem. Our recent study and publication emphasized the analysis of non-linear elasticity and elasto-plasticity with isotropic hardening, using a data-driven paradigm enhanced by tangent space and transition rules, based on structured data sets. To simulate plasticity, we augment the tangent space directly into the distance-minimizing data-driven formulation and classify the underlying data structure into subsets corresponding to different material behavior. We achieve the efficient material states by a fix-point iteration (*Fig. 14.2*). Using tangent space enables interpolation in regions of sparse data sampling, ensuring the internal states cohere with the data set.The data subset classification allows dealing with loading paths arising in inelasticity, avoiding the reliance on models for the evolution of history variables. We define transition rules to map the system's internal states to the various subsets. Consequently, the extended data-driven paradigm evaluates the closest point in the transitioned material data subset consistent with the problem's field equations and closest to the local tangential direction. In our latest publication [Ciftci and Hackl 2022], we investigated several numerical simulations, including a load-subjected plate with a hole (*Fig.14.3*), to show the convergence of the data-driven solution. The possibility of dealing with non-linearities and path dependency suggests dealing with more complex material behavior like finite strain, damage, and mixed hardening models. Moreover, the data-driven paradigm's growth proposes essential research areas in machine-learning methods, especially physics-informed neural networks. These networks can be trained to satisfy data and discover optimal solutions for allocated physics-governing equations by specifying suitable loss functions. Since the data-driven method skips the material modeling but still depends on solving governing equations, a merged formulation neural network method is possible.

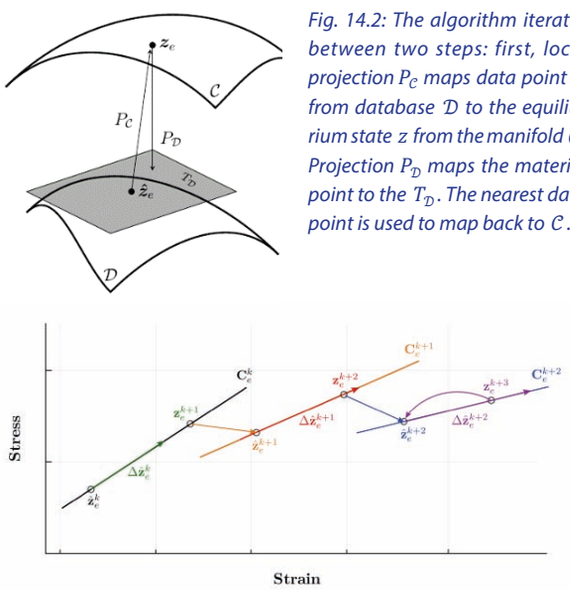


Fig. 14.2: The algorithm iterates between two steps: first, local projection $P_{\mathcal{C}}$ maps data point $\hat{z}$ from database $\mathcal{D}$ to the equilibrium state z from the manifold $\mathcal{C}$. Projection $P_{\mathcal{D}}$ maps the material point to the $T_{\mathcal{D}}$. The nearest data point is used to map back to $\mathcal{C}$.

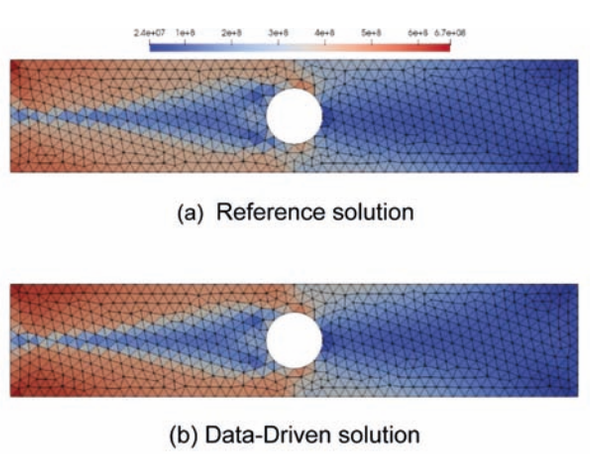


Fig. 14.3: Von Mises stress distribution at maximum loading at each integration point using a (a) J_2 -plasticity model and (b) the data-driven algorithm used on a sample containing 10^4 data points.

Influence of tissue degradation on a potential self-amplification of aneurysms

To investigate the effect of tissue degradation on the complex interplay of blood flow and tissue mechanics in aneurysms, an established damage model for arteries was implemented in SIMVASCULAR, a fluid-structure interaction (FSI) code for cardiovascular analysis. Based thereon, it was shown for the first time by [Wang et al 2021] that damage can be considered in FSI simulations using a monolithic solver approach. Based on this numerical framework, in [Wang et al 2022], patient-specific models of aneurysms were computationally analyzed in realistic boundary value problems and the distributions of the time-averaged wall shear stress (TAWSS) and the oscillatory shear index (OSI) over the aneurysm were computed. (*Fig.14.4*) shows exemplary results. The two quantities are considered significant for the risk of aneurysm growth. More precisely, a low TAWSS and a high OSI represent an increased risk of aneurysm development or progression. Simulations have shown that upon an already small tissue degradation, a relevant reduction of TAWSS and an increase of OSI were obtained. This implies that tissue degradation may contribute to a self-amplification of aneurysm progression. These findings could be reproduced for different patient-specific aneurysms, varying degradation intensities, heart rates and internal pressures.

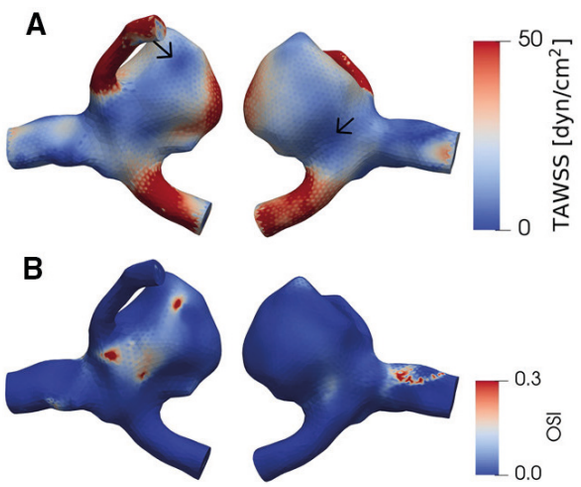


Fig. 14.4: Distribution of (A) time-averaged wall shear stress (TAWSS) and (B) oscillatory shear index (OSI) in a patient-specific aneurysm as a result of a full fluid-structure-interaction simulation. Results show that regions with low TAWSS and high OSI show an even lowered TAWSS and increased OSI upon already slight tissue degradation. This shows that the complex blood flow in combination with tissue degradation may lead to self-amplified aneurysm growth.

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[Wang et al 2021] H. Wang, D. Balzani, V. Vedula, K. Uhlmann, F. Varnik. On the potential self-amplification of aneurysms due to tissue degradation and blood flow revealed from FSI simulations. Frontiers in Physiology, 12:785780, 2021. doi: 10.3389/fphys.2021.785780.

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ICAMS

Publications

15. Publications

► Publications in Refereed Journals, Proceedings, and Books

L. Romaner, T. Pradhan, A. Kholtobina, R. Drautz, M. Mrovec
Theoretical investigation of the 70.5 mixed dislocations in body-centered cubic transition metals
Acta Materialia, 217, 117154, 2021

N. Volz, F. Xue, C. H. Zenk, A. Bezold, S. Gabel, A. P. Subramanyam, R. Drautz, T. Hammerschmidt, S. K. Makineni, B. Gault, M. Göken, S. Neumeier
Understanding creep of a single-crystalline Co-Al-W-Ta superalloy by studying the deformation mechanism, segregation tendency and stacking fault energy
Acta Materialia, 214, 117019, 2021

A. Neogi, R. Janisch
Twin-boundary assisted crack tip plasticity and toughening in lamellar γ-TiAl
Acta Materialia, 213, 116924, 2021

S. Iseni, M. Ramaswamy Guru Prasad, A. Hartmaier, K. Holeczek, N. Modeler, F. di Mare
Micro-, macromechanical and aeroelastic investigation of glass-fiber based, lightweight turbomachinery components
Asme Turbo Expo 2020: Power for land, sea and air, 10A, 14951, 2021

A. Obaied, F. Tang, I. Roslyakova, M. to Baben
"2 ½th" generation Calphad databases: Extrapolating heat capacities of elements and compounds to 0K
CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry, 75, 102352, 2021

L. Zhao, J. Zhang, J. Zhang, A. Hartmaier
Atomistic investigation of machinability of monocrystalline 3C–SiC in elliptical vibration-assisted diamond cutting
Ceramics International, 47, 2358, 2021

S. Lu, J. Zhang, Z. Li, J. Zhang, X. Wang, A. Hartmaier, J. Xu, Y. Yan, T. Sun
Cutting path-dependent machinability of SiCp/Al composite under multi-step ultra-precision diamond cutting
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Phase-field modeling of grain growth in presence of grain boundary diffusion and segregation in ceramic matrix mini-composites
Computational Materials Science, 190, 110295, 2021

E. Tamsen, D. Balzani
A general, implicit, finite-strain FE^2 framework for the simulation of dynamic problems on two scales
Computational Mechanics, 67, 1375, 2021

M. Shahmardani Firouzjah, N. Vajragupta, A. Hartmaier
Influence of crystal plasticity parameters on the strain hardening behavior of polycrystals
Crystals, 11, 1473, 2021

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Finite element modeling of brittle and ductile modes in cutting of 3C-SiC
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Geometry and flow properties affect the phase shift between pressure and shear stress waves in blood vessels
Fluids, 6, 378, 2021

H. Wang, D. Balzani, V. Vedula, K. Uhlmann, F. Varnik
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Frontiers in Physiology, 12, 785780, 2021

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Constitutive modeling of cyclic plasticity at elevated temperatures for a nickel-based superalloy
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On the role of pre-existing defects in influencing hardness in nanoscale indentations – insights from atomistic simulations
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Pair-exchange diffusion model for multicomponent alloys revisited
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P. Metsch, R. Schiedung, I. Steinbach, M. Kästner
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A mechanical analysis of chemically stimulated linear shape memory polymer actuation
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On the size effect of additives in amorphous shape memory polymers
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Physical Review B, 104, 64413, 2021

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Physical Review Materials, 5, 103801, 2021

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J. Jenke, A. N. Ladines, T. Hammerschmidt, D. G. Pettifor, R. Drautz
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M. Bruns, M. R. Hassani, F. Varnik, A. Hassanpour, S. V. Divinski, G. Wilde
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K. Ciftci, K. Hackl
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Computational Mechanics, 70, 425, 2022

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Modelling and Simulation in Materials Science and Engineering, 30, 35007, 2022

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Physical Review Materials, 6, 104411, 2022

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S. Li, N. Vajragupta, A. Biswas, W. Tang, H. Wang, A. Kostka, X. Yang, A. Hartmaier
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Surface and Coatings Technology, 445, 128730, 2022

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Experimental investigation of laser surface texturing and related biocompatibility of pure titanium
The International Journal of Advanced Manufacturing Technology, 119, 5993, 2022

M. Bruns, F. Varnik
Enhanced dynamics in deep thermal cycling of a model glass
The Journal of Chemical Physics, 156, 234501, 2022

V. Stieve, M. Blaszczyk, K. Hackl
Inverse modeling of cancellous bone using artificial neural networks
ZAMM - Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik, 102, 202100541, 2022

► Bachelor, Master, and PhD Theses

O. Aliyev
Analyse des Dämpfungsverhaltens von faserverstärkten Polymermatrix-Verbundwerkstoffen mit Hilfe der Finite-Elemente-Methode
Bachelor Thesis, Ruhr-Universität Bochum

D. El Lahib
Verdichterschaufeln aus faserverstärktem Kunststoff für Turbomaschinen
Bachelor Thesis, Ruhr-Univerisität Bochum

V. Lenz
Implementierung und Evaluation einer intuitiven Benutzeroberfläche für komplexes High-Performance Computing
Bachelor Thesis, Fernuniversität Hagen

T. Muslubas
Optimierung der mechanischen Belastbarkeit von Überspannungsableitern im GFK-Kreuzwickeldesign
Bachelor Thesis, Ruhr-Univerisität Bochum

N. Athanasopoulos
Atomistically-informed crystal plasticity simulations of hydrogen embrittlement in ferrite
Master Thesis, Ruhr-Universität Bochum

Y. Chiang
Prediction of anisotropic behavior for porous 316L stainless steel by machine learning methods
Master Thesis, Ruhr-Universität Bochum

S. Farzaneh Kalourazi
Python based automated data correlation on aluminum cast alloys
Master Thesis, Ruhr-Universität Bochum

E. Fedorov
Accelerated force field development using active learning: the case of advanced electrolytes for Li-ion batteries
Master Thesis, Ruhr-Universität Bochum

F. Frankus
Numerical investigation on the modalities of hydrogen-assisted crack growth in DCB specimen
Master Thesis, Ruhr-Universität Bochum

Z. Hamzeh
Finite element modelling of the influence of porosity in indentation tests
Master Thesis, Ruhr-Universität Bochum

M. U. Hassan
Influence of W-concentration on creep-behavior and phase stability in polycrystalline Ni-based superalloys
Master Thesis, Ruhr-Universität Bochum

W. Hu
Generative deep neural networks for x-ray diffractograms decomposition
Master Thesis, Ruhr-Universität Bochum

S. S. Hurain
Anisotropic grain growth in ceramics in presence of grain boundary segregations
Master Thesis, Ruhr-Universität Bochum

J. Jeon
Crystal structure and mechanical properties of Cr-rich hard phases of type M_7C_3 in Fe-based alloys - simulation and experimental validation
Master Thesis, Ruhr-Universität Bochum

M. Joulaian
Pyiron workflow for first-principles field evaporation calculations with applications to bcc metals
Master Thesis, Ruhr-Universität Bochum

S. Kumtamukkula
Exploring deep generative modeling approaches with 2D to 3D polycrystalline icrostructures generation
Master Thesis, Ruhr-Univerisität Bochum

Y. Lee
Prediciton of the load-path dependent bahavior of a polycrystalline material by micromechanical modeling
Master Thesis, Ruhr-Universität Bochum

M. M. Matsuo
Hybrid FEM-ML in open die forging process
Master Thesis, Ruhr-Universität Bochum

B. Medghalchi
Concentration-dependent finite temperature effects in metallic alloys
Master Thesis, Ruhr-Universität Bochum

M. Morales Cócera
Sampling equilibrium states in 2D Lennard-Jones systems with Boltzmann generators
Master Thesis, Ruhr-Universität Bochum

A. Oswal
Design and development of complex stressed polymer-metal hybrid structures
Master Thesis, TU Dortmund

A. W. Paiva do Nascimento
An optimized method to determine advanced yield surface initial parameters for sheet metal forming applications
Master Thesis, Ruhr-Univerisität Bochum

J. Schmidt
Prediction of Yld2004-18p anisotropic coefficients using ML methods
Master Thesis, Ruhr-Universität Bochum

A. Shetty
Machine-learning based surrogate modeling of indentation
Master Thesis, Ruhr-Univerisität Bochum

S. Sidrah
Scale-sensitive modeling of fracture and brittle-to-ductile transition in visco-plastic materials
Master Thesis, Ruhr-Universität Bochum

I. Sravani Dandu
Identification of mechanical properties from incremental indentation test
Master Thesis, Ruhr-Universität Bochum

A. Tiwari
Thermal stress calculation of SPS coatings by FEM analysis
Master Thesis, Ruhr-Universität Bochum

F. Valiente Dies
Development of a machine learning model to reconstruct 3D microstructures from 2D cuts
Master Thesis, Ruhr-Universität Bochum

M. Zar
FE simulation and surrogate modeling of soda-lime-silica glass glass bending process using the finite element method and Gaussian process regression
Master Thesis, Ruhr-Universität Bochum

A. Azócar Guzmán
Ab initio study of co-segregation effects of H and C at grain boundaries in ferritic steels
PhD Thesis, Ruhr-Universität Bochum

S. M. Benito
Design, implementation, and application of original methods of the microstructural characterization of powder metallurgy tool steels
PhD Thesis, Ruhr-Univerisität Bochum

A. Chauniyal
Deformation behavior of lamellar TiAl alloys – an atomistic study
PhD Thesis, Ruhr-Universität Bochum

M. Grabowski
Atomistic simulations of vacancy mobility in the γ – phase of Ni-based superalloys
PhD Thesis, Ruhr-Universität Bochum

A. Obaied
Developing state of the art materials informatics methods for Calphad modeling of multicomponent materials
PhD Thesis, Ruhr-Universität Bochum

M. Ramaswamy Guru Prasad
Microstructure-sensitive modeling of mechanical behavior of polycrystalline metals and superalloys
PhD Thesis, Ruhr-Universität Bochum

M. Rinaldi
Modelling magnetism from the electronic structure to continuum for iron and its alloys
PhD Thesis, Ruhr-Universität Bochum

R. Srinivas Varanasi
Mechanismsm of refinement and deformation of novel ultrafine-grained medium manganese steels with improved mechanical properties
PhD Thesis, Ruhr-Universität Bochum

S. Vakili
Multi-Phase-Field modelling of structure formation in metallic foams
PhD Thesis, Ruhr-Universität Bochum

V. Vardanyan
Molecular dynamics modeling of machining processes of composite materials
PhD Thesis, University of Kaiserslautern

H. Wang
Computational study of hemodynamic changes associated with morphology, deformability and degradation of blood vessels
PhD Thesis, Ruhr-Universität Bochum

ICAMS

Talks and Posters

16. Talks and Posters

▶ Invited Talks

08.01.2021
M. A. Stricker, E. Mak, B. Yin, W. Curtin
A neural network potential for magnesium and its application to prismatic cross-slip
Max Planck Institute for Iron Research, Düsseldorf, Germany

28.01.2021
Y. Liang, G. Díaz Leines, R. Drautz, J. Rogal
Identification of a multi-dimensional reaction coordinate for crystal nucleation in Ni_3Al
CECAM Mixed-gen Webinar, Lausanne, Switzerland, online event

17.02.2021
A. Grünebohm
New concepts for cooling: origins of the inverse electrocaloric effect
Virtual Colloquium IFC, Universidad Nacional Autonoma de Mexico, Mexico

20.04.2021
T. Hammerschmidt
Machine-learning the structural stability of intermetallic phases with domain knowledge of the interatomic bond
MRS Spring Meeting, Seattle, USA

18.05.2021
M. Qamar
Modelling carbon and its allotropes
SurMat Retreat, online event

01.06.2021
M. Mrovec, D. Smirnova, S. Starikov, T. Pradhan, M. Qamar, R. Drautz
Atomistic insights into microstructural defects and their role in H embrittlement
Thermec 2021, Vienna, Austria, online event

01.06.2021
T. Hammerschmidt
Formation of precipitates of topologically close-packed phases in Ni-base and Co-base superalloys
Thermec 2021, Vienna, Austria, online event

11.06.2021
R. Drautz
Atomic cluster expansion for accurate and transferable interatomic potentials
Multi-Scale Mechanics (MSM) group seminar, Groningen, The Netherlands

14.06.2021
G. Eggeler, L. Cao, A. Dlouhý, P. Thome, C. Somsen, K. Neuking
On the effect of stress state and crystallography on microstructural evolution in single crystal Ni-base superalloys
Creep 2021, online event

21.06.2021
M. A. Stricker, B. Yin, E. Mak, W. Curtin
What is materials informatics? An introduction and selected exampels from plasticity and metallurgy
RUB Physik Kolloquium, Ruhr-Universität Bochum, Germany

08.09.2021
M. A. Stricker, B. Yin, E. Mak, W. Curtin
What is materials informatics? An introduction and selected examples from plasticity and metallurgy
DGM Materials Week, online event

15.09.2021
R. Drautz
Atomic cluster expansion for accurate and transferable interatomic potentials
EUROMAT 2021, Graz, Austria, online event

27.09.2021
A. Grünebohm
Interplay of domain structure and phase transitions in ferroelectric $BaTiO_3$
DPG Meeting SKM21, online event

30.09.2021
I. Steinbach
3-D phase-field simulations to machine-learn 3-D features from 2-D microstructures
2021 International Conference on Phase-Field Method and Related Methods

06.10.2021
T. Hammerschmidt
Machine learning the structural stability of topologically close-packed phases
Intermetallics 2021, Bad Staffelstein, Germany

19.10.2021
I. Steinbach
Phase-field simulation of metal processing using the software library Openphase
International Symposium on Metal Processing, ISMP2021, Shenyang, China, online event

26.10.2021
R. Drautz
Atomic cluster expansion for bridging from electrons to materials properties
NHR Atomistic Simulation Center Inauguration Symposium, FAU Erlangen-Nürnberg, Germany, online event

08.11.2021
R. Drautz
Atomic cluster expansion for bridging from electrons to materials properties
EPFL Materials science and engineering (IMX) seminar series, Lausanne, Switzerland, online event

09.11.2021
A. Grünebohm
Hysteresis design of ferroelectric materials
25th German Female Physicists' Conference 2021, Universität Duisburg-Essen, online event

16.11.2021
A. Grünebohm
Interplay of domain structure, phase transitions and functional responses in ferroelectric $BaTiO_3$
Virtual Seminar Series "Time Man", Université de Lille, France, online event

22.11.2021
M. A. Stricker, B. Yin, E. Mak, W. Curtin, M. Ziemann, M. Walter, S. Weygand, P. Gruber, D. Weygand
Machine learning for plasticity
3rd Materials Chain International Conference (MCIC) 2021: Materials Discovery and Processing for Energy, Bochum, Germany, online event

14.12.2021
T. Hammerschmidt
Exploration of complex intermetallics by machine learning with domain knowledge
Exploiting machine learning in multiscale modelling of materials, Warwick, UK

14.12.2021
R. Khachaturyan
Impact of ultrafast field application on domain wall dynamics: a coarse-grained molecular dynamics study
Liège, Belgium

15.12.2021
I. Roslyakova, U. Nwachukwu, A. Obaied, O. Horst, M. A. Ali, I. Steinbach
Computer vision for analysis of microstructure evolution
MRM 2021, Yokohama, Japan, hybrid conference

19.12.2021
A. Grünebohm
New concepts for cooling: origins of the inverse electrocaloric effect
Shiraz University, Iran, online event

28.02.2022
R. Drautz
ACE of spades
TMS 2022, Anaheim, USA

03.03.2022
G. Eggeler
Nanoindentation of NiTi shape memory alloys
TMS 2022, Anaheim, USA

08.03.2022
R. Drautz
ACE of spades
Los Alamos National Laboratoy, USA

09.03.2022
R. Drautz
ACE of spades
CSRI - Sandia National Laboratories, USA

16.03.2022
R. Drautz
Atomic cluster expansion as a platform for constructing atomic scale models
Physical Symmetry-Aware Machine Learning of Interatomic Interactions and Properties of Materials, APS March Meeting, Chicago, USA

18.03.2022
R. Drautz
Automated parameterization of the atomic cluster expansion for predicting phase stability and mechanical properties
Large-Scale First Principles Atomistic Simulation: Recent Advances and New Challenges, Chicago, USA

21.03.2022
M. Qamar
ACE potential for C; parametrization and application
Atomic Cluster Expansion International Seminar Series, online event

24.03.2022
R. Janisch, A. Azócar Guzmán, A. P. Subramanyam, S. Vincent, J. Jeon, A. Hartmaier
Trapping of hydrogen at grain boundaries in ferritic steels – the role of grain boundary structure and composition
International Seminar Series on the Microstructure of Materials, online event

29.03.2022
J. Frenzel, O. Oluwaseyi, D. Piorunek, G. Eggeler
Microstructures, martensitic transformations and atomic mobilities in high entropy shape memory alloys
DGM workshop Functional Materials, Bochum, Germany

01.04.2022
R. Drautz
ACE of spades
School of Physics / CRANN, Trinity College Dublin, Ireland, online event

01.04.2022
R. Drautz
ACE of spades
Condensed matter seminar series, Physics Division at Lawrence Livermore National Laboratory, USA, online event

13.04.2022
R. Drautz
Atomic cluster expansion and application to modelling of materials
BiGmax Workshop 2022, Ruhr-Universität Bochum, Germany

24.04.2022
R. Drautz
Atomic cluster expansion for fast and accurate interatomic potentials
Machine Learning in Chemical and Materials Sciences Center for Nonlinear Studies, Los Alamos National Laboratory, USA, online event

11.05.2022
R. Drautz
Atomic cluster expansion for fast and accurate interatomic potentials
Theoretical chemistry colloquium, Ruhr-Universität Bochum, Germany

16.05.2022
J. Frenzel
Fundamentals of shape memory alloys
SMST 2022 Workshop, Carlsbad, California, USA

19.05.2022
J. Frenzel, A. Wieczorek, G. Eggeler
Effect of alloy compositions and microstructures of NiTi-based shape memory alloys on elastocaloric cooling performance
SMST 2022 Workshop, Carlsbad, California, USA

07.06.2022
M. A. Stricker
Materials informatics – introduction, application to metal plasticity
Seminar Series on Data-Driven and Artificial Neural Network / Machine Learning Methods for Computational Material Modeling and Simulation, RWTH Aachen, Germany

08.06.2022
D. Balzani, D. Wingender
Simulation of crack propagation in hard metal microstructures
Ruhr-Universität Bochum, Germany

13.06.2022
T. Hammerschmidt
Machine-learning material properties with domain knowledge of the interatomic bond
Physics Colloqium, Ruhr-Universität Bochum, Germany

28.06.2022
I. Steinbach, O. Shchyglo, I. Roslyakova, V. Mohles, M. A. Ali, D. K. Nerella, H. F. Salama, C. Eberl, U. Krupp, M. Ackerman
Intelligent-data-guided process design for fatigue-resistant bainitic steel: iBain
The 8th International Conference on Solid-Phase Transformations in Inorganic Materials, online event

04.07.2022
R. Janisch, A. Azócar Guzmán, A. Hartmaier
Hydrogen enhanced decohesion in ferritic steels – a reassessment of the first-principles cohesive zone model
European Solid Mechanics Conference 2022 (ESMC 2022), Galway, Ireland

11.07.2022
R. Drautz
Atomic cluster expansion: some lessions learned from Francois Ducastelle
Journee Francois Ducastelle, Ecole des Mines de Paris, France

05.08.2022
M. A. Stricker, B. Yin, E. Mak, W. Curtin
Fitting and using machine-learned interatomic potentials for plasticity
World Congress on Computational Mechanics WCCM, Yokohama, Japan, online event

28.08.2022
M. A. Stricker
Materials informatics: introduction, applications, and future
Materials Chain International Conference on Future Energy Materials and Systems 2022, Ruhr-Universität Bochum, Germany

29.08.2022
Y. Lysogorskiy, A. Bochkarev, M. Rinaldi, M. Qamar, M. Mrovec, R. Drautz
Atomic cluster expansion for materials modeling
Materials Chain International Conference on Future Energy Materials and Systems 2022, Ruhr-Universität Bochum, Germany

01.09.2022
R. Drautz
Atomic cluster expansion for accurate and fast interatomic potentials
AFLOW Seminar, Duke University, Durham, USA, online event

07.09.2022
P. Thome, M. Schneider, E. J. Payton, V. A. Yardley, G. Eggeler
On the transition between lath to plate martensite in Fe-Ni alloys
ESOMAT 2022, Ankara, Turkey

13. 09. 2022
A. Grünebohm
Optimizing the electrocaloric effect by ab initio based simulations: the role of microstructure
Calorics 2022, Cambridge UK

13. 09. 2022
R. Janisch, A. Neogi, A. Chauniyal
Crack twin-boundary interactions in lamellar γ-titanium aluminide alloys
Materials Structure and Micromechanics of Fracture 10 (MSMF 10), Brno, Czech Republic

14. 09. 2022
A. Grünebohm
Quasi-martensitic transitions in polar perovskites
Electronic driving forces of martensitic phase transitions, Hamm, Germany

28. 09. 2022
G. Eggeler
On the importance of chemistry, crystallography and microstructure for the high temperature strength of single crystal Ni-base superalloys
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28. 09. 2022
J. Frenzel, G. Eggeler
Structural and functional fatigue in shape memory alloys
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

29. 09. 2022
A. Grünebohm
Double hysteresis loops in Pb-fre ferroelectrics by microstructure design
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

03. 10. 2022
F. Varnik, H. Dumlu, E. Mahmoudinezhad Zirdehi, G. Eggeler
Effects of additive molecules on shape memory effect in polymers: a combined experimental and computer simulation study
10th Multiscale Materials Modelling Conference (MMM10) 2022, Baltimore, Maryland, USA

11. 10. 2022
R. Drautz
From DFT to ACE
CECAM Flagship Workshop Charting large materials dataspaces: AI methods and scalability, Grenoble, France

20. 10. 2022
A. Grünebohm
Origins of the inverse electrocaloric effect
Lecture series of the Graduiertenkolleg IGK 2495, FAU Erlangen-Nürnberg, Germany

04. 11. 2022
R. Drautz
ACE of spades
Festkolloquium Computergestützte Materialwissenschaft: Von der virtuellen Realität zu experimentellen Fakten, TU Darmstadt, Germany

04. 12. 2022
F. Varnik
Chemically triggered shape memory polymers: molecular modelling and experiments
Advanced Materials Discussion Series at Shiraz University, Iran

09. 12. 2022
F. Scholz
3D characterization of dendritic solidification and crystal mosaicity in Ni-based single crystal superalloys
Journée Scientifique FERMI, Paris, France

► Contributed Talks and Posters

17.02.2021
I. Roslyakova, S. Zomorodpoosh, M. A. Ali, A. Obaied, I. Steinbach
Artificial materials intelligence (AMI) to accelerate discovery of novel superalloys
ML & AI @ RUB Research Exchange Workshop, Bochum, Germany

25.02.2021
J. Frenzel
Using shape memory alloys for cooling processes
Materials for Energy Conference, UA Ruhr, online event

11.03.2021
R. Drautz
Atomic cluster expansion for accurate and transferable interatomic potentials
Workshop Workflows for Atomistic Simulations, online event

16.03.2021
L. Heep, D. Bürger, C. Bonnekoh, P. Wollgramm, A. Dlouhý, G. Eggeler
SFB/TR 103 research on the influence of crystallography on creep of Ni-base single crystal superalloys
Adelbodener Werkstoffseminar, Adelboden, Switzerland

15.03.2021
F. Scholz, J. He, O. M. Horst, P. Thome, G. Eggeler, B. Gault, J. Frenzel
Crystal mosaicity and local alloy chemistry of low angle grain boundaries in Ni-based superalloys
TMS 2021, online event

17.03.2021
P. Thome, F. Scholz, A. Richter, J. Frenzel, G. Eggeler
Using the new rotation vector base line electron back scatter diffraction (RVB-EBSD) method to characterize single crystal cast microstructures
TMS 2021, online event

19.03.2021
Y. Liang, G. Díaz Leines, R. Drautz, J. Rogal
Enhanced sampling of structural phase transformations using a neural network based path collective variable
APS March Meeting 2021, online event

22.03.2021
I. Roslyakova, S. Zomorodpoosh, M. A. Ali, A. Obaied, I. Steinbach
Application of artificial intelligence to the design of a novel superalloy
Materials Data Science for Accelerating Materials Discovery and Design, Bochum, Germany

24.03.2021
F. Varnik
Decelerated aging in metallic glasses by low temperature thermal cycling
Online-Tagung der Deutschen Physikalischen Gesellschaft

06.04.2021
Y. Liang, G. Díaz Leines, J. Rogal, R. Drautz
Sampling structural phase transformations in tungsten
1st Virtual Workshop on Computational Materials Science, online event

07.04.2021
M. Qamar
Data analysis for parameterizing a carbon potential
MPI-E Retreat, online event

08.06.2021
T. Hammerschmidt, A. N. Ladines, A. P. Subramanyam, J. Jenke, M. D. Forti, Y. Lysogorskiy, R. Drautz
Machine learning structural and functional properties of transparent conducting oxides
ICAMS Advanced Discussions, Bochum, Germany

15.06.2021
M. A. Ali, O. Shchyglo, I. Steinbach
Phase-field coupled strain gradient crystal plasticity model to study high temperature creep in Ni-based superalloys
15th International Conference on Creep and Fracture of Engineering Materials and Structures, online event

15.06.2021
M. Shahmardani Firouzjah, A. Hartmaier
Low cycle fatigue modeling of a single crystal nickel -based superalloy at different temperature ranges
15th International Conference on Creep and Fracture of Engineering Materials and Structures, online event

15.06.2021
S. Starikov
Two-scale simulation of plasticity in bcc metals: combination of atomistic simulation and dislocation dynamics
15th International Conference on Creep and Fracture of Engineering Materials and Structures, online event

16.06.2021
D. Bürger, M. Sirrenberg, K. Neuking, A. Dlouhý, G. Eggeler
The role of elementary dislocation processes in medium temperature creep of single crystal Ni-base superalloys
Creep 2021, online event

16.06.2021
L. Heep, D. Bürger, C. Bonnekoh, P. Wollgramm, A. Dlouhý, G. Eggeler
How do deviations from <100> target tensile directions affect creep in the low temperature high stress creep regime (750°C, 800 MPa)
Creep 2021, online event

29.06.2021
S. Starikov, D. Smirnova, M. Mrovec, R. Drautz
Atomistic simulation of bulk and grain boundary diffusion in iron
17th International Conference on Diffusion in Solids and Liquids, Malta, online event

06.08.2021
M. A. Stricker, B. Yin, E. Mak, W. Curtin
Machine learning a neural network interatomic potential for magnesium
ICAMS Advanced Discussion, Bochum, Germany

26.08.2021
M. A. Stricker
Materials informatics overview, applications, and vision
ICAMS Retreat, online event

13.09.2021
A. A. Kraych, A. Bochkarev, Y. Lysogorskiy, M. Mrovec, R. Drautz
Investigation of tungsten plasticity using atomic cluster expansion
EUROMAT 2021, Graz, Austria, online event

13.09.2021
O. M. Horst, S. Ibrahimkhel, J. Streitberger, N. Wochmjakow, P. Git, F. Scholz, P. Thome, R. Singer, J. Frenzel, C. Körner, G. Eggeler
On the influence of alloy composition on creep behavior of Ni-based single crystal (SX) superalloy
Superalloys 2021, online event

15.09.2021
R. Namdar, H. Safari, S. Hosseini, D. Thévin, F. Varnik
Lattice Boltzmann simulations of reacting flows in small-scale static and moving beds of particles with complex shapes
CRC-TRR 287 Workshop 2022, Hannover, Germany

15.09.2021
A. Bochkarev, A. A. Kraych, Y. Lysogorskiy, M. Mrovec, R. Drautz
Automated parameterization of the atomic cluster expansion
EUROMAT 2021, Graz, Austria, online event

15.09.2021
M. A. Stricker, B. Yin, E. Mak, W. Curtin
Prismatic slip in magnesium with a neural network potential
EUROMAT 2021, Graz, Austria, online event

16.09.2021
S. Starikov
Two-scale simulation of plastic deformation in bcc metals: combination of atomistic simulation and dislocation dynamics
EUROMAT 2021, Graz, Austria, online event

16.09.2021
S. Starikov, D. Smirnova, T. Pradhan, M. Mrovec, R. Drautz
Atomistic study of hydrogen behavior in Fe in presence of crystal defects
EUROMAT 2021, Graz, Austria, online event

27.09.2021
M. A. Stricker, W. Curtin
Prismatic slip in magnesium with a neural network potential
DPG Meeting SKM21, online event

28.09.2021
T. K. Schmalofski, M. Kroll, H. Dette, R. Janisch
An efficient sequential approach to sample the grain boundary parameter space
84th Annual Meeting of DPG of the Condensed Matter Section, online event

08.10.2021
M. Qamar
ML potentials of carbon; review of datasets and fitting procedures
POTENTIALS project seminar, online event

21.10.2021
S. Starikov, V. Tseplyaev, M. Mrovec
Two-scale simulation of plastic deformation in bcc metals: combination of atomistic simulation and dislocation dynamics
Materials Science and Technology 2021, Columbus, USA, online event

01.11.2021
I. Pietka, M. D. Forti, A. P. Subramanyam, A. Burakovskaya, R. Drautz, T. Hammerschmidt
Modelling of extended defects in superalloys
Young Researchers' Meeting, Kloster Irsee, Germany

02.11.2021
L. Qin
Atomic simulation of diffusion and segregation in Ni-based superalloys
Young Researchers' Meeting, Kloster Irsee, Germany

22.11.2021
A. Grünebohm
Hysteresis design of ferroelectric materials
3rd Materials Chain International Conference (MCIC) 2021: Materials Discovery and Processing for Energy, Bochum, Germany, online event

06.12.2021
A. Dimou, P. Hirel, A. Grünebohm
The effect of Sr on the mobility of 180° domain walls in $BaTiO_3$
4th Young Materials Researchers' Day, Ruhr-Universität Bochum, Germany

06.12.2021
I. Pietka, R. Drautz, T. Hammerschmidt
Partitioning of transition metals to the γ and γ' phase of Co-based superalloys
4th Young Materials Researchers' Day, Ruhr-Universität Bochum, Germany

06.12.2021
L. Qin
Atomic simulation of segregation and diffusion on γ/γ' interface in Ni-based superalloys
4th Young Materials Researchers' Day, Ruhr-Universität Bochum, Germany

06.12.2021
M. Sirrenberg, D. Bürger, P. Thome, K. Neuking, G. Eggeler
High-temperature plasticity of single crystal Ni-base superalloys
4th Young Materials Researchers' Day, Ruhr-Universität Bochum, Germany

06.12.2021
T. K. Schmalofski, R. Janisch, M. Kroll, H. Dette
Sampling the parameter space of grain boundaries with a sequential sampling technique – atomistics meets statistics
4th Young Materials Researchers' Day, Ruhr-Universität Bochum, Germany

28.02.2022
F. Scholz, P. Thome, J. Frenzel, G. Eggeler
3D characterization of competitive dendrite growth and on the role of low angle grain boundaries during solidification of single Crystal Ni-based superalloys
TMS 2022, Anaheim, California, USA

02.03.2022
M. Sirrenberg, D. Bürger, A. B. Parsa, G. Eggeler
On the influence of γ'-particle size on the yield stress anomaly in Ni-base single crystal superalloys
TMS 2022, Anaheim, California, USA

13.03.2022
O. Oluwaseyi, J. Frenzel, G. Eggeler
Atomic mobilities and martensitic transformations in NiTi-Based shape memory alloys with chemical gradients
ICOMAT 2022, online event

14.03.2022
P. Thome, M. Schneider, E. J. Payton, V. A. Yardley, G. Eggeler
In-depth EBSD investigation of spatially coupled crystallographic properties in binary Fe-Ni alloys
ICOMAT 2022, online event

17.03.2022
J. Frenzel, A. Paulsen, G. Eggeler
Recent progress on Ti-Ta-based high temperature shape memory alloys
ICOMAT 2022, online event

23.03.2022
M. Qamar, M. Mrovec, Y. Lysogorskiy, A. Bochkarev, R. Drautz
Parametrization of atomic cluster expansion potential for carbon
International ACE Seminar, online event

28.03.2022
P. Thome, F. Scholz, G. Eggeler, J. Frenzel
Single crystal cast microstructures characterized by the RVB-EBSD method
TMS 2022, Anaheim, California, USA

17.05.2022
T. Hammerschmidt
On the role of refractory d-shell elements in SFB/TR 103
MRD Industry Day 2021, Bochum, Germany

17.05.2022
O. Oluwaseyi, J. Frenzel, G. Eggeler
Effects of off-stoichiometric compositions on microstructures and martensitic phase transformations in Ni-Cu-Pd-Ti-Zr-Hf high entropy shape memory alloys
SMST 2022 Workshop, Carlsbad, California, USA

21.05.2022
O. Oluwaseyi, J. Frenzel, G. Eggeler
Effects of chemical complexity on microstructures, martensitic transformations and atomic mobilities
HEAs Symposium, Ruhr-Universität Bochum, Germany

02.06.2022
M. Qamar, M. Mrovec, Y. Lysogorskiy, A. Bochkarev, R. Drautz
Modelling nano-scale carbon materials with quantum accuracy
SurMat Retreat, Akademie Biggesee, Attendorn, Germany

09.06.2022
R. Drautz
Atomic interactions - classical to machine learning interatomic potentials
From Electrons to Phase Diagrams, Ruhr-Universität Bochum, Germany

13.06.2022
D. Wingender, D. Balzani
Combining finite cells and eigenerosion for an efficient simulation of ductile crack propagation through metal matrix composites
IUTAM International Conference of Solid Mechanics (ICONSOM), Alghero, Italy

20.06.2022
T. K. Schmalofski, M. Kroll, R. Janisch, H. Dette
An efficient sequential approach to sample the grain boundary parameter space
MRD Materials Day 2022, Ruhr-Universität Bochum, Germany

28.06.2022
S. Starikov
Macroscopic characteristics of plastic deformation in bcc metals described through dislocation mobility properties
19th ICSMA, Metz, France

28.06.2022
A. B. Parsa, D. Bürger, L. Cao, G. Eggeler
Exploring the influence of different stress states and the transition towards topological inversion
19th ICSMA, Metz, France

30.06.2022
G. Eggeler, F. Fox, J. Pfetzing, P. Thome, E. P. George
Alloy chemistry and size effect: a micromechanical study of fcc high entropy alloys
19th ICSMA, Metz, France

05.08.2022
D. Wingender, D. Balzani
Voxel-based simulations of ductile crack propagation through metal matrix composite microstructures based on eigenerosion and finite cells
World Congress on Computational Mechanics (WCCM), Yokohama, Japan, online event

24.08.2022
R. Drautz
Atomic cluster expansion for accurate and transferable interatomic potentials
Psi-k 2022, Lausanne, Switzerland

24.08.2022
Y. Lysogorskiy, A. Bochkarev, M. Mrovec, R. Drautz
Active learning strategies for atomic cluster expansion (ACE) models
Psi-k 2022, Lausanne, Switzerland

25.08.2022
T. Hammerschmidt, M. D. Forti, A. Burakovskaya, R. Drautz
Atomic-environment descriptors with domain-knowledge of the interatomic bond
Psi-k 2022, Lausanne, Switzerland

05.09.2022
L. Qin
Atomistic simulation of diffusion in γ'-strengthened Co-based superalloys
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

05.09.2022
S. Teng, A. Grünebohm
Impact of point defects on the ferroelectric phase diagram: a molecular dynamics study on the defect arrangements
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

05.09.2022
T. K. Schmalofski, M. Kroll, R. Janisch, H. Dette
An efficient method to access the grain boundary parameter space with atomistic simulations
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

05.09.2022
N. Stötzel, J. Frenzel, G. Eggeler
Coupled functional structural fatigue of NiTi-based shape memory alloys – degradation mechanisms, damage accumulation and fatigue lives
ESOMAT 2022, Ankara, Turkey

06.09.2022
M. Qamar, M. Mrovec, Y. Lysogorskiy, A. Bochkarev, R. Drautz
Transferable atomic cluster expansion potential for carbon
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

06.09.2022
S. Starikov, A. A. Kraych, M. Mrovec
Macroscopic characteristics of plastic deformation described through dislocation mobility properties
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

07.09.2022
A. Dimou, P. Hirel, A. Grünebohm
Pinning of domain walls by strontium inclusions in $BaTiO_3$
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

07.09.2022
E. Ibrahim, Y. Lysogorskiy, M. Mrovec, R. Drautz
Atomic cluster expansion: a universal machine learning potential for magnesium
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

07.09.2022
Y. Liang, M. Mrovec, Y. Lysogorskiy, R. Drautz
Atomic cluster expansion for the Ag-Pd system
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

08.09.2022
L. Hsu, F. Wendler, A. Grünebohm
The relation between electrocaloric effect and non-collinear electric fields: a coarse-grained case study of $BaTiO_3$
DPG Meeting of the Condensed Matter Section 2022, Universität Regensburg Germany

09.09.2022
J. Frenzel, D. Piorunek, O. Oluwaseyi, G. Eggeler
Microstructures and martensitic transformations in high entropy shape memory alloys – effects of chemical complexity and off-stoichiometry
ESOMAT 2022, Ankara, Turkey

19.09.2022
D. Kozinov, N. Miska, D. Balzani
Using machine learning for efficient computational homogenization of variable artificial microstructure morphologies
Annual Congress of the International Association of Applied Mathematics and Mechanics (GAMM), Aachen, Germany

19.09.2022
F. Werner, A. Richter, F. Scholz, P. Thome, P. Git, C. Körner, J. Frenzel
Effects of single crystal growth techniques on dendritic microstructures and small angle misorientation defects in Ni-based superalloys
EuroSuperalloys 2022, Bamberg, Germany

19.09.2022
J. Hunfeld, J. Kiese, A. Kostka, G. Laplanche, H. Sommer, C. Somsen, G. Eggeler
Design and creep of a new polycrystalline Ni-base superalloy
EuroSuperalloys 2022, Bamberg, Germany

20.09.2022
L. Heep, D. Bürger, C. Bonnekoh, P. Wollgramm, A. Dlouhý, G. Eggeler
Crystallographic loading directions and creep of Ni-base SXs
EuroSuperalloys 2022, Bamberg, Germany

20.09.2022
L. Qin
First-principles study of solute interactions and partitioning in Ni-based superalloys
EuroSuperalloys 2022, Bamberg, Germany

20.09.2022
T. Jogi, M. A. Stricker
High-Temperature creep behaviour of Ni-base superalloys using parametric climb functions in discrete dislocation dynamics
EuroSuperalloys 2022, Bamberg, Germany

20.09.2022
S. Teng, C. N. Anabaraonye, L. Hsu, M. Marathe, A. Grünebohm
Impact of defects and microstructure on the ferroelectric phase diagram: ab initio based molecular dynamics studies
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

21.09.2022
M. Sirrenberg, D. Bürger, S. Guth, G. Eggeler
Assessing the high temperature strength of Ni-base SX
EuroSuperalloys 2022, Bamberg, Germany

22.09.2022
P. Thome, F. Scholz, A. Richter, J. Frenzel, G. Eggeler
3D dendrite growth in Ni-base SXs analyzed using microstructure informatics
EuroSuperalloys 2022, Bamberg, Germany

25.09.2022
O. Oluwaseyi, J. Frenzel, G. Eggeler
Atomic mobilities and martensitic transformations in NiTi-based shape memory alloys with chemical gradients
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

27.09.2022
O. Gülbay, J. Wang, M. Ackermann, S. Wesselmecking, U. Krupp
Data-driven characterization of microstructural, phase transformation and mechanical properties of bainitic steel
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28.09.2022
A. Chauniyal, M. A. Stricker
Estimiating geometrically necessary dislocations from Kikuchi patterns
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28.09.2022
A. Chauniyal, R. Janisch
How interfaces dictate plasticity in nanolamellar alloys: an atomistic investigation using lamellar TiAl as a case study
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28.09.2022
A. Chauniyal, R. Janisch
Influence of pre-existing defects on nanoindentation: insights from atomistic simulations
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28.09.2022
J. Wang, A. Hussain, U. Krupp, S. Wesselmecking
idCarl: intelligent digital Computational advanced research laboratory
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28.09.2022
R. Janisch, A. Neogi
Crack twin-boundary interactions in lamellar TiAl alloys
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

28.09.2022
S. Starikov, A. A. Kraych, M. Mrovec
Macroscopic characteristics of plastic deformation described through dislocation mobility properties
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

29.09.2022
G. Tolooei Eshlaghi, G. Egels, S. Weber, A. Hartmaier
Data-based characterization of metastable austenitic steels
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

29.09.2022
M. A. Stricker, M. Ziemann, M. Walter, S. Weygand, P. Gruber, D. Weygand
Data fusion from modeling and experiments: dislocation structures in the strain gradient of torsion
Materials Science and Engineering (MSE) Congress 2022, Darmstadt, Germany

05.10.2022
J. Schmidt, A. Biswas, N. Vajragupta, A. Hartmaier
Data-oriented description of texture-dependent anisotropic plastic material behavior
MMM10, Baltimore, USA

06.10.2022
R. Schiedung, M. Ode
Simulating sintering of solidstate battery materials with phase-field
MMM10, Baltimore, USA

26.10.2022
S. Starikov
Macroscopic characteristics of plastic deformation in bcc refractory metals described through dislocation mobility properties
NuMat Conference, Ghent, Belgium

28.10.2022
M. Qamar, M. Mrovec, Y. Lysogorskiy, A. Bochkarev, R. Drautz
Atomic cluster expansion for quantum-accurate simulations for carbon
5th Young Materials Researchers' Day, Bochum, Germany

03.11.2022
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 – Intelligent-data-guided process design for fatigue-resistant steel components with bainitic microstructure
Plattform MaterialDigital (PMD) Vollversammlung, Berlin, Germany

04.11.2022
D. Wingender, D. Balzani
Finite cell method and eigenerosion for the efficient simulation of ductile crack propagation through metal matrix composites
African Conference on Computational Mechanics (AFRICOMP), Cape Town, South Africa

14.11.2022
A. Grünebohm
Interplay of ferroelectric domain walls, phase transitions and functional responses
MaWi colloqium, TU Darmstadt, Germany

17.11.2022
A. Dimou
Stability of dopants in $BaTiO_3$
R. Cohen, Carnegie Institute, Washington DC, USA

ICAMS

Seminars and other Lectures

17. Seminars and other Lectures

▶ Joint Seminar Series of ICAMS and the Institute for Materials

21.01.2021
Machine learning and computational mechanics: the natural next step
C. J. Cyron
TU Hamburg, Germany

28.01.2021
AMANDA - Line 1: A prototype line for automated materials innovation
C. Brabec
Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

20.05.2021
Paving the way towards three dimensional microstructure and strain characterization during in situ deformation
C. Kirchlechner
Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

10.06.2021
Accelerating materials science for clean energy production, storage and utilization
H. Stein
Karlsruhe Institute of Technology, Ulm, Germany

17.06.2021
Advanced, in situ and cryo-EM for materials research
B. Butz
Universität Siegen, Germany

01.07.2021
Ab initio-accurate large-scale molecular dynamics using machine-learning interatomic potentials
M. Hodapp
Skoltech, Moscow, Russia

08.07.2021
Prediction and optimization of antiferroelectric materials
J. Iñiguez
Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg

15.07.2021
Hydrogen in nanoscale metals under contraint conditions
A. Pundt
Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

16.12.2021
Metallurgy in Colombia: current state and challenges towards sustainability
L. Mujica Roncery
Pedagogical and Technological University of Colombia, Tunja, Colombia

13.01.2022
Development of high modulus steels: maturation from combinatorial screening towards industrial application
H. Springer
RWTH Aachen, Germany

20.01.2022
Efficient discovery of novel high strength high entropy alloys by multiscale modelling
F. Maresca
University of Groningen, The Netherlands

27.01.2022
Magnetic materials for efficient energy conversion
O. Gutfleisch
TU Darmstadt, Germany

03.02.2022
Fatigue behaviour caught between material physics based damage phenomena and influences from process history
M. Zimmermann
TU Dresden, Germany

12.05.2022
Revision of the Cr-Mn phase diagram after in situ powder neutron diffraction
J. Joubert
Université de Paris, France

19.05.2022
Tailoring the functionality of transition metal oxide surfaces and interfaces for energy conversion applications
R. Pentcheva
Universität Duisburg-Essen, Duisburg, Germany

09.06.2022
Machine learning for accelerated molecular simulations and discovery
P. Friederich
Karlsruhe Institute of Technology, Germany

23.06.2022
New methods and opportunities across the scales – on complex crystals, lattice defects and deformation damage
S. Korte-Kerzel
RWTH Aachen, Germany

07.07.2022
Electrocatalyst dissolution assessment in fuel cells and water electrolysers
S. Cherevko
Forschungszentrum Jülich, Germany

21.07.2022
Study protocols that enable data science-informed materials manufacturing design
J. L. Carter
Case Western Reserve University, Cleveland, USA

27.10.2022
Materials-based innovations for the supply and use of hydrogen
T. Hosenfeldt
Schaef er AG, Herzogenaurach, Germany

17.11.2022
Computational materials engineering with active learning
M. Todorovic
University of Turku, Finland

24.11.2022
Data-driven chemical understanding with geometrical and quantum-chemical bonding analysis
J. George
Friedrich-Schiller-Universität Jena, Germany

01.12.2022
Partial dislocation densities and character in different slip modes from X-ray powder
T. Ungár
Eötvös Loránd University, Budapest, Hungary

► Seminars and other Lectures

17.02.2021
Platform Material Digital: workflow management via pyiron
M. R. Hassani
MPIE Düsseldorf, Germany

01.03.2021
Phase-coherent caloritronics with topological superconductors
B. Sothmann
Universität Duisburg-Essen, Duisburg, Germany

13.07.2021
Hydrogen effects on the mechanical behavior of Fe alloys at small scale
J. Duarte
MPIE Düsseldorf, Germany

08.09.2021
Computation-experiment-simulation approach to predict perovskite solar cell efficiency as well as stability from atomic scale
M. Kanani
Shiraz University, Iran

22.10.2021
Combinatorial materials science, data science, and machine learning applied to complex materials discovery and science
J. Schroers
Yale University, New Haven, USA

28.10.2021
Understanding electrochemical energy storage in transition metal oxides containing structural water
V. Augustyn
North Carolina State University, Raleigh, USA

04.11.2021
From interface modifications of thermo-electric materials towards tellurium-free thermoelectric devices
K. Nielsch
IFW Dresden, Germany

05.11.2021
Digitalization of the battery manufacturing process
A. Franco
Université de Picardie Jules Verne, Amiens, France

09.12.2021
Nanocrystal aerogels – macroscopic materials with nanoscopic properties
N. Bigall
Leibniz Universität, Hannover, Germany

10.12.2021
Quantitative visualisation of surface structure-reactivity: next generation design of materials and processes
P. Unwin
University of Warwick, Coventry, U.K.

17.12.2021
Insights into electrodes via reaction kinetic modeling
U. Krewer
Karlsruher Institut für Technologie, Germany

14.02.2022
Chiral superconductivity with enhanced quantized Hall responses in moiré transition metal dichalcogenides
M. Scherer
Ruhr-Universität Bochum, Germany

07.11.2022
Computational materials research in an industrial context
E. Wimmer
Materials Design S.A.R.L., Montrouge, France

14.11.2022
Ab initio chemical engineering for searching new material system for Li-ion battery cathode with high-performance capacity and structural stability: fully ab initio DFPT approach
M. Kanani
Shiraz University, Iran

29.11.2022

Descriptor-based microstructure characterization and reconstruction: DMCR and MCRpy

P. Seibert
TU Dresden, Germany

ICAMS

Teaching

18. Teaching

► MSS lecture courses summer term 2021

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

J. Kundin
The CALPHAD method

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

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

R. Drautz
Quantum mechanics in materials science

► MSS lecture courses winter term 2021/22

A. Grünebohm, M. Mrovec
Advanced atomistic simulation methods

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
Documenting and communicating science

G. Eggeler
Elements of microstructure

T. Li
Introduction to 3-dimensional materials characterization techniques

A. Grünebohm
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

I. Roslyakova
Practical applications of material informatics with R

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

I. Steinbach
Solidification processing

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

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

► Block course on modelling – University of Oxford, 15.11.2021–19.11.2021

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

► MSS lecture courses summer term 2022

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

J. Kundin
The CALPHAD method

A. Hartmaier
Computational plasticity

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Data-driven materials science

T. Hammerschmidt, R. Janisch
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A. Grünebohm, M. Scherer
Physics of complex phase transitions in solids

R. Drautz
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Y. Lysogorskiy
Advanced statistical methods in materials science

R. Drautz
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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. Li
Introduction to 3-dimensional materials characterization techniques

F. Körmann
Introduction to quantum mechanics

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

M. Stricker
Materials informatics

R. Janisch
Multiscale mechanics of materials

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

I. Steinbach
Solidification processing

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

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

► Block course on modelling – University of Oxford, 14.11.2022 – 18.11.2022

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

► ICAMS Graduate School

PhD seminar: 18.02.2021

Part II: The phase-field approach, block course from 13.–14.04.2021

PhD seminar: 20.07.2021

Part III: Micromechanical and macroscopic modelling, block course from 01.– 02.09.2021

PhD seminar: 08.02.2022

PhD seminar: 30.09.2022

ICAMS

ICAMS Members 2021 and 2022

19. ICAMS Members 2021 and 2022

▸ Staff at ICAMS

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

Figure 19.1 shows the development of ICAMS staff numbers through the past eleven years. By the end of 2010 about 57 people were working at ICAMS. From 2011 to 2014 this number increased and by the end of 2014 almost 90 people worked at ICAMS. Since the end of the start-up funding in 2013, staff numbers decreased due to a smaller number of industry projects.

Since 2017, the number of employees has leveled off at around 80. The majority of ICAMS scientists hold a degree in engineering and materials science, followed by degrees in physics, mathematics or computer science and chemistry (*Fig. 19.2*). This educational diversity of our research staff provides the basis for ICAMS' interdisciplinary research.

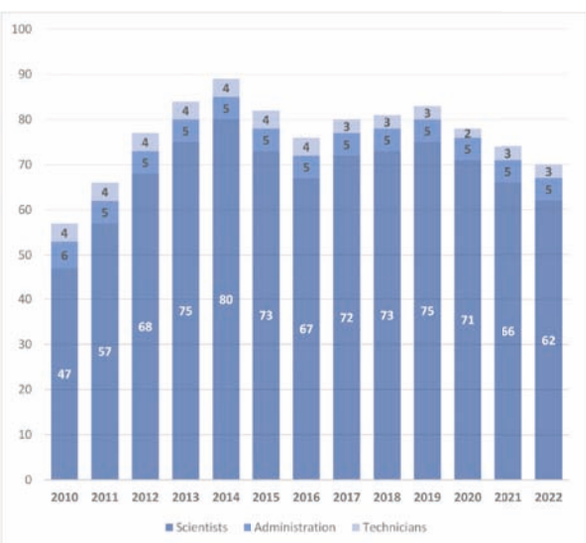


Fig. 19.1: Development of ICAMS staff from 2010 to 2022.

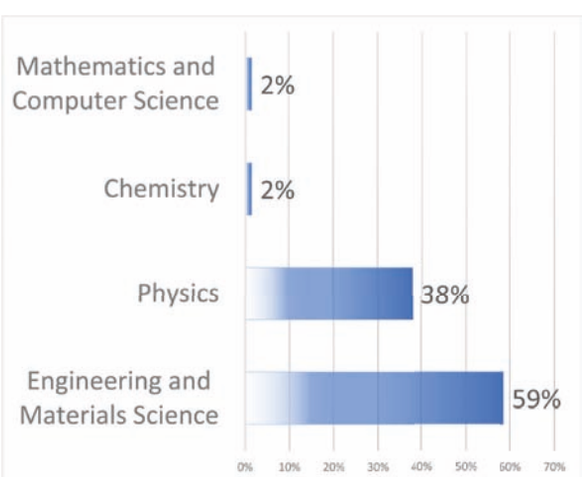
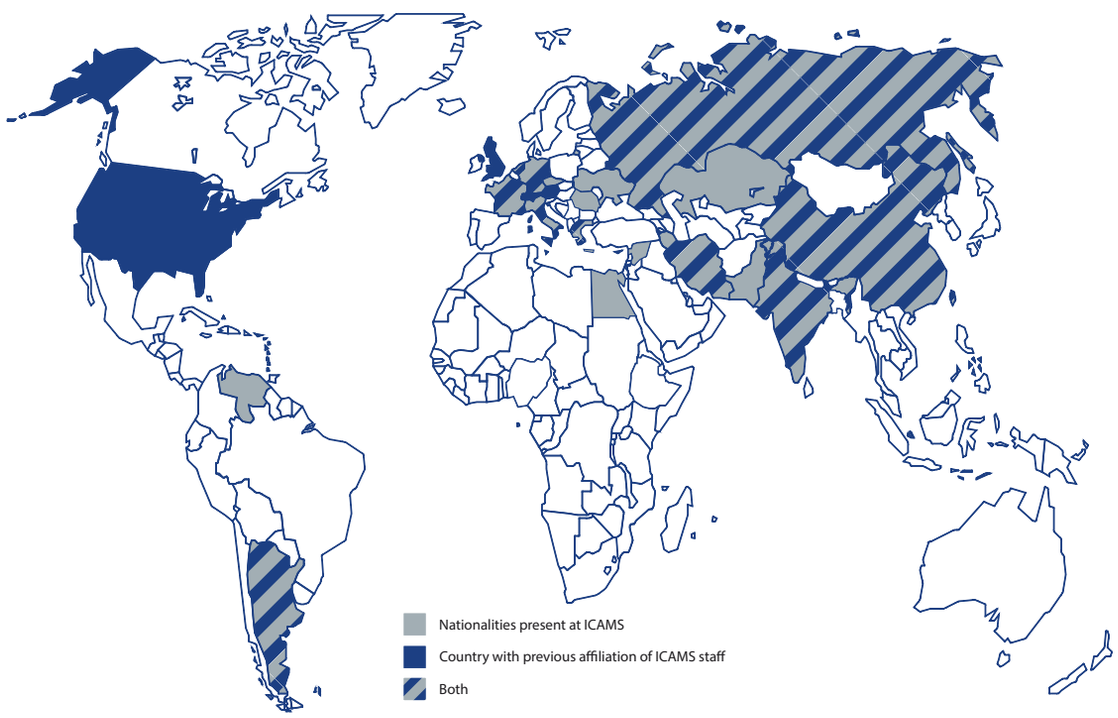


Fig. 19.3: Breakdown of first degree of ICAMS researchers in 2021/2022.

In 2021 and 2022 researchers from 23 different countries were working at ICAMS (see grey areas in *Fig. 19.3*). 34% of the ICAMS staff is of German and 66% of foreign nationality. For ICAMS, it is of vital importance to attract talented scientists from leading research institutions worldwide.

Figure 19.3 gives an overview of the countries and institutions of origin of the current ICAMS researchers. 13 of the 39 institutions are located in Germany, 14 in other EU countries and 12 in non-EU countries. Staff members are encouraged to stay in contact with their previous research institutions, thus helping ICAMS to establish a tight network of international collaborations.



Previous affiliations of ICAMS members

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National University of General San Martín

Austria
Technical University of Vienna

China
Central South University, Changsha
Tianjin University

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

Germany
AICE, Aachen
BASF, Ludwigshafen
Fraunhofer IWM, Freiburg
Friedrich-Alexander Univ., Erlangen-Nürnberg
Ruhr-Universität Bochum
RWTH Aachen
TU Darmstadt
TU Dortmund
Universität Bayreuth
Universität Duisburg-Essen

Greece
University of Ioannina

India
Indian Institute of Science, Karnataka

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

The Netherlands
TU Delft

Russia
Kazan Federal University
JIHT Moskow

Switzerland
EPFL, Lausanne

Taiwan
National Chiao Tung University

United Kingdom
University of Oxford

USA
University of Rochester (NY)

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.

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Continuum Mechanics

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IT System Administration
IT Administration

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ICAMS

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20. Guests and Visitors

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