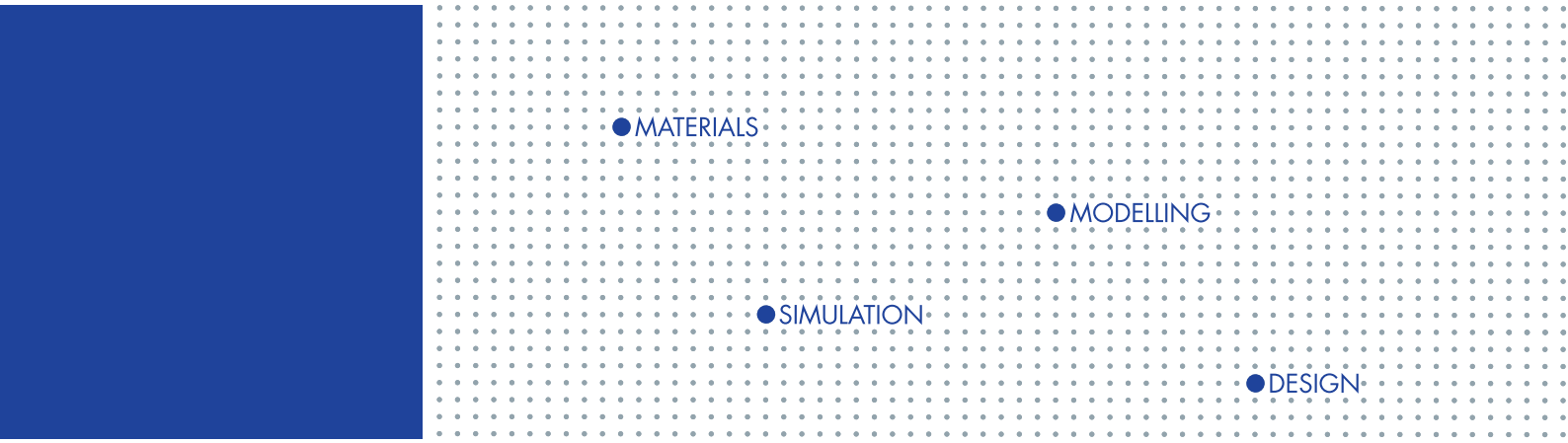
Scientific Report 2014



ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS

Scientific Report 2014

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Preface

More than ever before, materials with new and unprecedented functionality, superior structural stability, or increased corrosion and fatigue life time are the focal point of scientific research. These materials are deemed to be crucial for future advancements of modern technology. Therefore, predictive modelling and simulation of materials forms a basic necessity for knowledge-driven design of materials and processes. Although aspects of Integrated Computational Materials Engineering (ICME) are used in many industries, the development of reliable models of materials, based on microstructure and composition, is still a challenge to meet.

The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) is dedicated to the development of these models. Since its foundation in 2008 ICAMS has established itself among the world's leading institutes focusing on the development and application of simulation tools for multi-scale materials modelling. Within the approach taken by ICAMS, the different length scales relevant for materials (macroscopic behaviour of materials, mesoscale descriptions of microstructures, atomistic structures providing information on phase stability and transformation kinetics, electronic modelling) are bridged by an interdisciplinary team of scientists from engineering, materials science, chemistry, physics, information technology and mathematics.

Two significant collaborative research projects, covering all scales relevant for materials and involving the active participation of all ICAMS departments, reached a matured state in 2014. The design of "Damage Tolerant Microstructures in Steel" is in the focus of a project financed by two of ICAMS' industrial partners. It aims at a full theoretical understanding of the deformation mechanisms in low carbon tempered martensitic steels. One particular objective of our research is to understand the limits of deformability beyond which damage and failure occur and to predict microstructures and processing routes to push those limits further towards higher strength and increased deformability.

The second essential research activity focusses on the development of new concepts in single crystal technology and is integrated into a DFG-funded Collaborative Research Centre (SFB/Transregio 103 "From Atoms to Turbine Blades – a Scientific Approach for Developing the Next Generation of Single Crystal Superalloys"). Within this Collaborative Research Centre, five ICAMS based projects shape the core of the project group "Scale-bridging modelling and simulation" with strong interdepartmental links.

Furthermore, the department for Scale-bridging Thermodynamic and Kinetic Simulation collaborates with all of ICAMS' "Advanced Study Groups" within the DFG-funded Priority Program 1714 "Chemomechanics". This Priority Program, coordinated by ICAMS-representative Prof. Ingo Steinbach, started in September 2014 and investigates the interplay of mechanical and chemical forces in metals and polymers.

ICAMS' numerous activities and accomplishments in national and international research collaborations during 2014 are presented in this Scientific Report. Together with our sponsors, partners and all our members to whom we are much obliged, ICAMS will continue to pursue the development of predictive multi-scale materials simulations.

Ingo Steinbach
Managing Director
(until 31.3.2015)

Ralf Drautz
Managing Director
(from 1.4.2015)

Alexander Hartmaier
Director

Contents

ICAMS in 2014

2. ICAMS in 2014

For ICAMS, 2014 was the first year after the initial start-up funding period. The change from start-up funding to a regular scientific institute at the Ruhr-Universität Bochum meant that the role of ICAMS within the university had to be re-defined and that ICAMS' financial structure changed completely. The main focus of our work in 2014 was therefore on the successful continuation of ICAMS in a new setting. In the following, a brief account of ICAMS' activities during 2014 is given. The transition from the start-up period did not affect the research at ICAMS.

The departmental structure of ICAMS has not changed after the start-up phase. The ICAMS departments and Advanced Study Groups (ASGs) providing the expertise required for modelling and experiments across the length scales are summarised in *section 3*. Thereby, each department and ASG has its own specific focus and strength.

Project groups specialised on topics that are of broad interest to ICAMS foster cross-departmental interactions and bring together researchers who work on different aspects of the same or a related topic. The project groups are headed by two or three group leaders. *Section 3* gives a summary of the project groups and the project group leaders.

The work of ICAMS is annually reviewed by the ICAMS scientific advisory board. Its members *(see section 3)* are national and international experts from the field of materials science with a background in industrial or academic research. Five members represent the Ruhr-Universität Bochum. Prof. Dierk Raabe has been elected chairman at the board meeting in July 2014.

Research at ICAMS

Research at ICAMS is summarised in the following chapters of this Scientific Report. Here, only two large collaborative projects are briefly described as these two projects integrate researchers from all three ICAMS departments.

The ICAMS Demonstrator Project

The ICAMS demonstrator project on damage tolerant microstructures in steel may be seen as a continuation of the start-up phase, with funding provided by ThyssenKrupp Steel Europe and Benteler Steel/Tube. Researchers in the three ICAMS departments develop the foundations for first-principles-based optimisations of steel. This includes high-throughput density functional theory calculations, magnetic interatomic potentials for modelling (e.g., carbon segregation to dislocations), phase-field models for martensite and crystal plasticity, as well as experimental work.

SFB/Transregio 103

The Collaborative Research Centre/Transregio 103 "From Atoms to Turbine Blades – a Scientific Approach for Developing the Next Generation of Single Crystal Superalloys" focuses on the scientific basis for the next generation of Nickel and Cobalt-based superalloys for high-temperature applications in gas turbines. The Collaborative Research Centre/Transregio 103 started in 2012 and is funded by the German research foundation (DFG). The Collaborative Research Centre is a joint

activity of the universities in Bochum and Erlangen and headed by Prof. Gunther Eggeler at the Ruhr-Universtät Bochum. It comprises six projects on modelling and simulation, of which five are led by ICAMS researchers. The Collaborative Research Centre/Transregio may be extended for a total duration of up to 12 years; the review for the continuation period 2016-2020 will take place in June 2015.

Publications

In 2014 ICAMS researchers published 79 articles in peer-reviewed journals. In addition, the Advanced Study Groups listed 22 papers related to ICAMS. *Fig. 2.1* shows the number of publications and citations with ICAMS members (without ASGs) as authors since 2008 according to Thomson Reuters' Web of Science. The number of publications shows a characteristic oscillation according to the typical three-year-duration of our research projects.

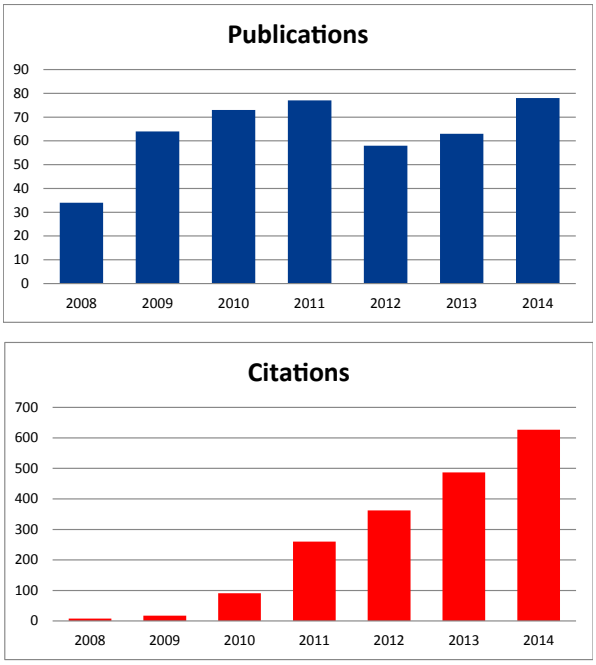

Figure 2.1: ICAMS' publications and citations (without ASGs) since 2008 according to Thomson Reuters' Web of Science.

Workshops and conferences, outreach

ICAMS organised and contributed to the organisation of several workshops and conferences in 2014. The ICAMS Advanced Discussions in July were reorganised, with external speakers, highlight talks from ICAMS members and a plenary disputation on "Theory meets Application".

Further events organised with the involvement of ICAMS:

- PFM 2014, August 2014, State College, Pennsylvania, USA
- Modelling and Simulation of Superalloys, September 2014, Bochum, Germany
- 14th Discussion Meeting on Thermodynamic Alloys, September 2014, Brno, Czech Republic
- ADIS 2014, October 2014, Ringberg, Germany.

Teaching

300 applications for the ICAMS Master's Course 'Materials science and simulation' were received in 2014. About fifty students were admitted, and twenty of them eventually took up their studies in the winter semester of 2014. In total, ten students completed their Master's degree, most of them moved on to PhD positions in Germany, but also in the USA or other countries. The re-accreditation of the course is planned for 2016.

Staff numbers and Finances

Staff numbers were not affected by the transition from the start-up phase to the continuation of ICAMS as an institute at the Ruhr-Universität Bochum. In 2014 about three quarters of the ICAMS staff where financed by third- party funding and approximately one quarter by central funds of the Ruhr-Universität Bochum. As salaries and costs associated directly to staff, such as travel expenses, constituted by far the largest expenditure of ICAMS, this also implies that ICAMS' income remains approximately constant after the start-up phase. Chapter 16 provides a detailed summary of the development of staff numbers in the past years. In 2014 80% of the acquired third-party funds came from public funding agencies like the DFG and 20% stemmed from industry.

The Ruhr-Universität Bochum contributes the core staff of ICAMS, i.e., the three ICAMS professors, 10 scientific staff members, i.e. the group leaders, the central coordination office, as well as the secretaries and IT technicians. Furthermore, the RUB provides the office facilities and operates the ICAMS computer cluster Vulcan.

Figure 2.2: ICAMS' Advisory Board Meeting.

Figure 2.4: Superalloys tutorials and workshop.

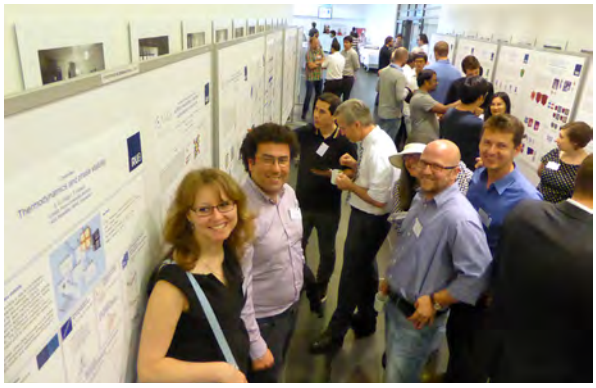

Figure 2.3: ICAMS' Advisory Board Meeting/Advanced Discussions - poster session.

Figure 2.5: ICAMS' students at the CIP Pool.

Organisation of ICAMS

3. Organisation of ICAMS

Board of Directors

Scientific Advisory Board

>> ICAMS Departments

Atomistic Modelling and Simulation
Chair: Prof. Dr. Ralf Drautz

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

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

High Performance Computing in Materials Science
Chair: Dr. Godehard Sutmann

ICAMS Project Groups

>> Advanced Study Groups

Modelling
Chair: Prof. Dr. Jörg Neugebauer

Input Data and Validation
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Processing and Characterization
Chair: Prof. Dr.-Ing. Wolfgang Bleck

Diffusion and Microstructure Analysis
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>> Board of Directors

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Prof. Dr. Alexander Hartmaier	Department Micromechanical and Macroscopic Modelling
Dr. Rebecca Janisch	Representative of the Scientific Staff
Niklas Caesar	Representative of the Non-Scientific Staff
Bonny Dongre	Students' Representative

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>> ICAMS Project Groups

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Deformation Mechanisms and Phase Transformations	Dr. Anxin Ma Dr. Oleg Shchyglo Jun.-Prof. Victoria Yardley
Kinetics of Phase Transformations	Dr. Jutta Rogal Dr. Robert Spatschek
Thermodynamics and Phase Stability	Dr. Suzana G. Fries Dr. Tilmann Hickel
Transport and Response	Dr. Georg Madsen Dr. Fathollah Varnik

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Department Atomistic Modelling and Simulation AMS

4. Department Atomistic Modelling and Simulation

Prof. Dr. Ralf Drautz

Research

The Department Atomistic Modelling and Simulation develops and applies models for bridging from the electronic through the atomistic scale to elementary processes of microstructural evolution. The focus of the research is thereby on,

1. the coarse graining of the electronic structure from density functional theory into a tight-binding representation that allows for a chemically intuitive analysis of bond formation and makes simulations with thousands of atoms possible,

2. the derivation of effective interatomic interactions from the tight-binding approximation and the application of the resulting bond-order potentials in atomistic simulations with millions of atoms as well as in the analysis of structural trends in alloys and steels,

3. the extension of the time-scale of atomistic simulations to the prediction of elementary processes of microstructural evolution, such as diffusion, segregation and phase transformation.

Models and parameterizations obtained in the Department Atomistic Modelling and Simulation serve as input for simulations that are carried out in the Department for Scale Bridging Thermodynamic and Kinetic Simulations and the Department Micromechanical Modelling of Materials Behaviour. The Department Atomistic Modelling co-ordinates the project groups 'Light elements and deformation mechanisms', 'Kinetics of phase transitions' and 'Transport and response'. For the development of high-throughput density-functional-based methods, simplified models of the electronic structure and large scale atomistic simulations, we collaborate closely with the Advanced Study Group Modelling at the Max-Planck-Institut für Eisenforschung.

Structure

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

- Simplified models of the electronic structure (Dr. Georg Madsen)

- Bond-order potential development and large-scale atomistic simulations (Dr. Thomas Hammerschmidt)

- Atomistic simulation of the kinetics of phase transformations (Dr. Jutta Rogal)

The three research groups are presented on the following pages, their interactions and role within ICAMS is explained schematically in *Fig. 4.1*.

Teaching

For the ICAMS Master´s course 'Materials Science and Simulation', the department coordinates the teaching activities on the electronic and atomistic modelling hierarchies. The Department AMS also contributes to teaching in the Departments of Physics and Astronomy and Mechanical Engineering at the Ruhr-Universität Bochum. As a Visiting Professor at the University of Oxford, Ralf Drautz contributes regularly to teaching in the Department of Materials at Oxford.

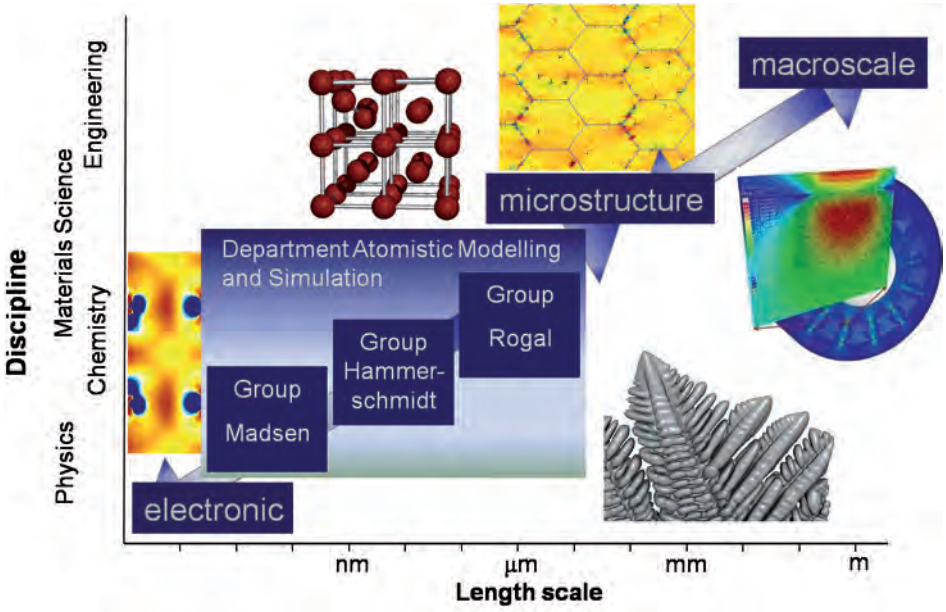

Fig. 4.1: Hierarchy of materials modelling and disciplines involved (from D.G. Pettifor, 1991), including a schematic representation of the research focus of the Department Atomistic Modelling and Simulation. The three research groups Madsen, Hammerschmidt and Rogal form a coherent link from the electronic length scale to the microstructural modelling hierarchy.

AMS

4.1 Simplified Models of the Electronic Structure

Group leader:
Dr. Georg Madsen

Group members:
Dr. Ingo Opahle
Dr. Sandip Bhattacharya
Ankita Katre
Robin Stern
Jingliang Wang

Dr. Georg Madsen's group is working on the development and application of electronic structure methods. The current focus is on method development, light elements in steel, transport properties such as thermal and electric conductivity, and high-throughput investigation of thermoelectric materials.

The research group presently has six members. Dr. Ingo Opahle is working on magneto caloric materials within the SPP1589 program of the DFG. Ankita Katre is a PhD student of the IMPRS graduate-school. She is working on thermal conductivity in nano-structured materials. Jingliang Wang is working within the Demonstrator project on segregation to grain boundaries in martensitic steels. Robin Stern is working on carrier controlling defects in Half-Heusler alloys and simplified models of thermal conductivity. Dr. Sandip Bhattacharya joined the group in February 2014. He is working on the discovery of new *pd*-bonded alloys for thermoelectric applications. In 2014 Dr. Chandan Bera left the group for a permanent position at the Institute of Nano Science and Technology, Mohali, India. Furthermore, N. S. Harsha Gunda left the group for a PhD position at the University of California, Santa Barbara.

Innocuous, low-cost and efficient thermoelectrics

Thermoelectric materials provide an environmentally friendly avenue to generate electricity. However, current state of the art thermoelectrics are either expensive, poisonous, or both. Recently we have identified tin sulfide (SnS) as an efficient novel thermoelectric system, based on a high-throughput (HT) study of binary sulfides. With a HT defect engineering study, we furthermore identified monovalent cations Li^+ and Ag^+ as probable p-dopants. Our experimental collaborators at IMRA measured the Seebeck coefficient and conductivities of Ag-doped SnS and found the resulting power factor to be an order of magnitude higher than that previously reported in literature.

The measurements for Li^+-doped SnS indicated poor transport properties, contrary to the theoretical predictions. We investigated two ubiquitous effects that can decrease the hole concentrations, namely the formation of coupled defect clusters and the oxidation of the dopant, as possible explanation of this disagreement. We identified that oxidation of the dopant limits the chemical potential of Li, thereby drastically reducing the carrier concentration. On the other hand, Ag is resistant to oxidation and therefore Ag-doped SnS has high power factors. This work serves as a comprehensive guide to achieve *p*-doped SnS and a road-map to the efficient discovery of new thermoelectric materials.

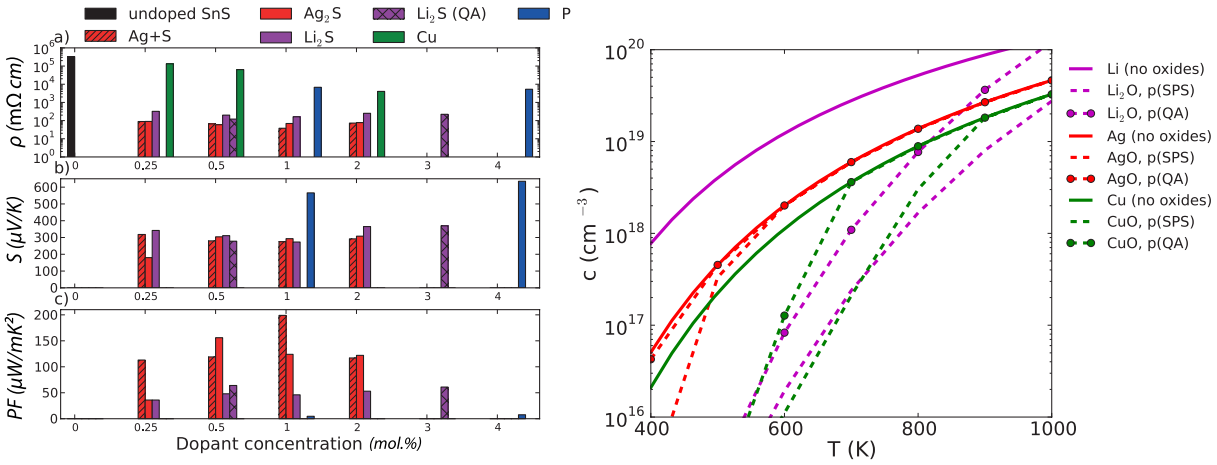

Fig. 4.2: Measurements for thermoelectric properties of p-doped SnS (left). Oxidation of the dopant drastically reduces the carrier concentration in Li and Cu-doped SnS, which directly corresponds to the experimental measurements (right). SnS doping with Ag is, however, resistant to oxidation for T>600 K. Collaborators: Gilles Dennler, IMRA Europe S.A.S.

Thermal management in nano-structured materials

Due to miniaturisation of electronic devices, improvement in their operating speeds, and advancements in the fabrication techniques, it is now possible to build complicated electronic circuits at the nanoscale. However, these factors have also made heat dissipations very critical, resulting in shorter lifetimes of electronic components and limiting their operational frequencies. Thermal management in the electronic devices is thus becoming crucial for further technological advancement.

We have studied thermal transport in one such class of technologically important materials, nano-structured zinc-chalcogenides based on the phonon Boltzmann transport equation (BTE). It is seen that in ZnS, two-thirds of the heat is carried by phonons with a mean-free path of more than 1 μm. This makes the thermal conductivity strongly influenced by the interaction of the phonons with defects, dislocations, grain boundaries, vacancies and other impurities. Furthermore, the influence of the nano-structure is strongly dependent on the respective materials. As seen in *Fig. 4.2*, zinc-chalcogenides show thermal conductivity cross-over with reduction in length scales, i.e., ZnSe and ZnTe have similar thermal conductivity in bulk, whereas ZnSe and ZnS thermal conductivities converge at the nanoscale.

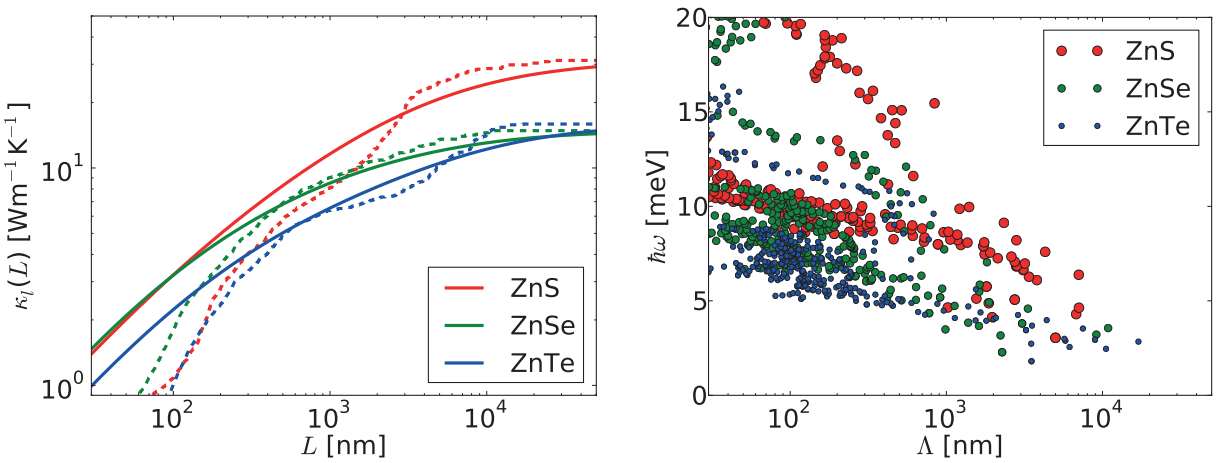

Fig. 4.3: Thermal conductivity of zinc-chalcogenides with nano-structure size (L) (left). MFP (Λ) distribution of phonons in zinc-chalcogenides (right).

Modelling the thermal conductivity is done in collaboration with Dr. Atsushi Togo at Kyoto University and Dr. Natalio Mingo at CEA Grenoble. Furthermore, we collaborate with Tao Wang and Prof. Alexander Hartmaier associated with the Department Micromechanical and Macroscopic Modelling (MMM) at ICAMS.

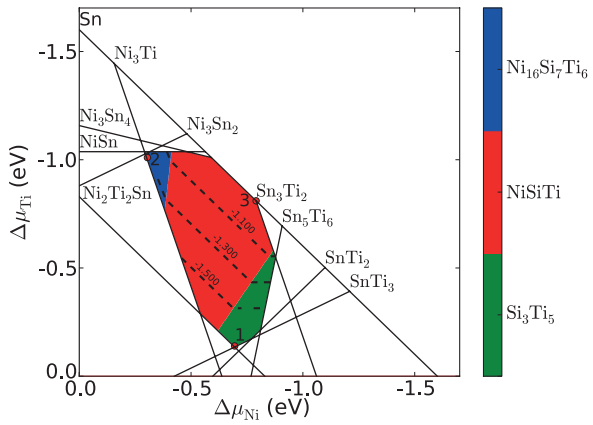

Fig. 4.4: Stability range for Si doping of the HHA NiTiSn.

High-throughput investigation of half-Heusler alloys

Half-Heusler alloys are an interesting class of materials for several different applications. The performance of a thermoelectric material is among other factors determined by the carrier concentration of the material, which can be manipulated by doping with electron-accepting or electron- donating atoms. The theoretical investigation of potential dopants is computationally intensive, because a number of constraints, such as the possibility of the formation of competing phases (*Fig. 4.4*), have to be taken into account. Furthermore, the number of possible locations for the dopant grows with more complicated structures.

We have developed a high-throughput framework in which we combine open access databases, such as materialsproject.com and AFLOW with automatised DFT calculations to efficiently identify potential dopants that optimise the carrier concentration and enhance the thermoelectric performance of half-Heusler alloys.

The project is carried out in collaboration with Dr. Wolf Eckhard Müller (Deutsches Zentrum für Luft- und Raumfahrt, Köln) and Prof. Alfred Ludwig (Institut für Werkstoffe, Ruhr-Universität Bochum).

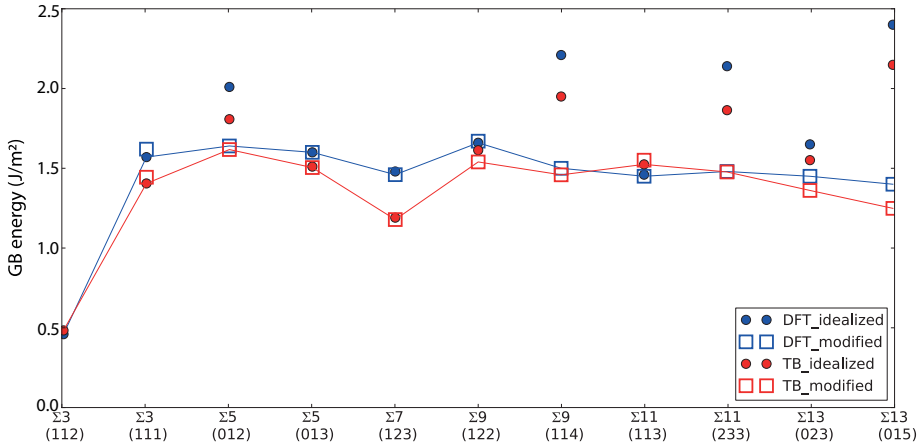

Fig. 4.5: Comparison between TB and DFT-calculated GB energies.

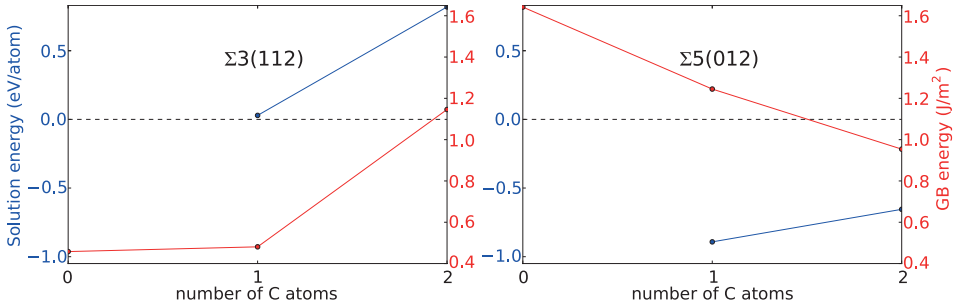

Fig. 4.6: Solution energy of carbon at GBs and GB energy variation with C concentration.

Grain boundary segregation in Martensitic steels

Based on previous calculations on different grain boundaries (GBs) in bcc-Fe using density functional theory (DFT), we modified our current tight-binding (TB) model for iron. By introducing a repulsive core term to the TB energy functional, we reasonably reproduced the GB energies as calculated by DFT. While DFT calculations are restricted to a few hundred atoms, the developed TB model makes the characterisation of larger systems possible. We attempted to characterise the twist GBs which possess the similar misorientation angles between adjacent variants in martensite. One example of that is the frequently observed [011]/60^{o} misorientation, which is close to that of twist GB ∑33(225)[011] within coincidence site lattice model.

We chose two representative GBs, ∑3(112) and ∑5(012), to study the effect of C on the GB energies with DFT calculations. It can be seen that C atoms tend to segregate to less stable GB and help to lower the GB energy (*Fig. 4.6*). The stable GB ∑3(112) is thus expected to show significantly lower C segregation than the other GBs.

The project is carried out within the Demonstrator project, where we collaborate with Dr. Rebecca Janisch and Jun.-Prof. Victoria Yardley.

AMS

4.2 Bond-Order Potentials and Large-Scale Atomistic Simulations

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Dr. Miroslav Čák
Hamid Reza Hajiyani
Jan Jenke
Dr. Jörg Koßmann
Alvin Ladines
Sebastian Schreiber
Ning Wang

The research group "Bond-Order Potentials and Large-Scale Atomistic Simulations", led by Dr. Hammerschmidt, focuses on predictive large-scale atomistic simulations by effective models of the interatomic interaction. This requires the development of robust parameterisations that overcome the limited reliability of existing models. To this end, the group develops, implements and parameterises analytic bond-order potentials (BOPs) derived from electronic-structure theory. These activities are complemented by high-throughput density-functional theory (DFT) calculations and the construction of empirical structure maps.

Current topics include (i) the interaction of dislocations in iron with point defects and interfaces, (ii) the stability and light-element solubility of intermetallic phases in steels and in single-crystal superalloys, (iii) the melting behaviour of refractory metals, (iv) the structural and electrochemical properties of transition-metal-based battery materials, (v) as well as the identification of trends in the stability in p-d- and d-d-bonded systems. Current members of the research group are Dr. Jan-Michael Albina, Dr. Arthur Bialon, Dr. Miroslav Čák, Hamid Reza Hajiyani, Jan Jenke, Dr. Jörg Koßmann, Alvin Ladines, Sebastian Schreiber and Ning Wang. Abdullah Hariri, student of the Master´s course MSS, carried out a student project in 2014.

Dr. Jan-Michael Albina (in close collaboration with Robert Bosch GmbH) investigates the structural stability of high-energy Ni-Co-Mn oxides for Li-ion batteries by high-throughput DFT calculations. This allows, e.g., to determine the structural stability of the Li-Mn-O system during dis-/charge in different environments, mimicked by chemical potentials (*Fig. 4.7*).

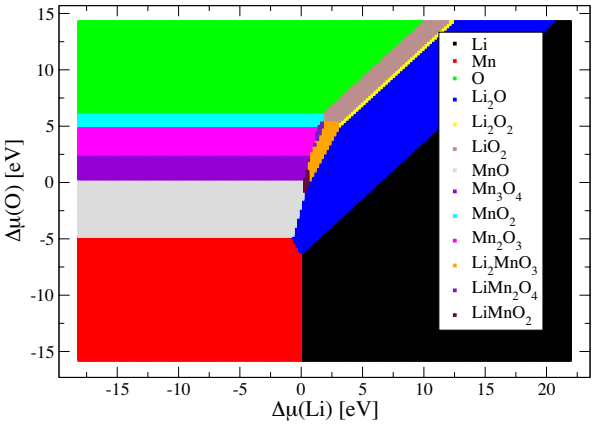


Fig. 4.7: Structural stability in the Li-Mn-O system as a function of the Li and O chemical potential. The colours show the stability regions for the various phases (Jan Albina).

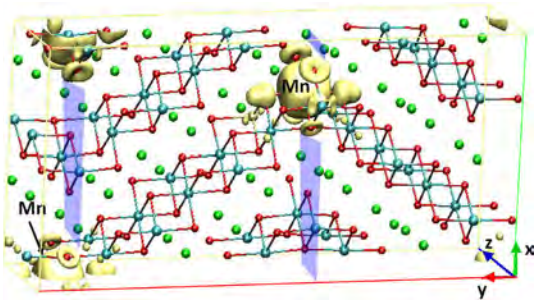


Fig. 4.8: Symmetric tilt grain-boundary in $LiCoO_2$ with iso-surface of charge-density for Mn doping atom in grain-boundary plane (Hamid-Reza Hajiyani).

These activities are complemented by the research of Hamid Reza Hajiyani (PhD student within the DFG priority program SPP1473 WeNDeLIB) on the trends of alloying and grain-boundaries in olivine-phosphate and layered-oxide cathode materials for Li-ion batteries (*Fig. 4.8*).

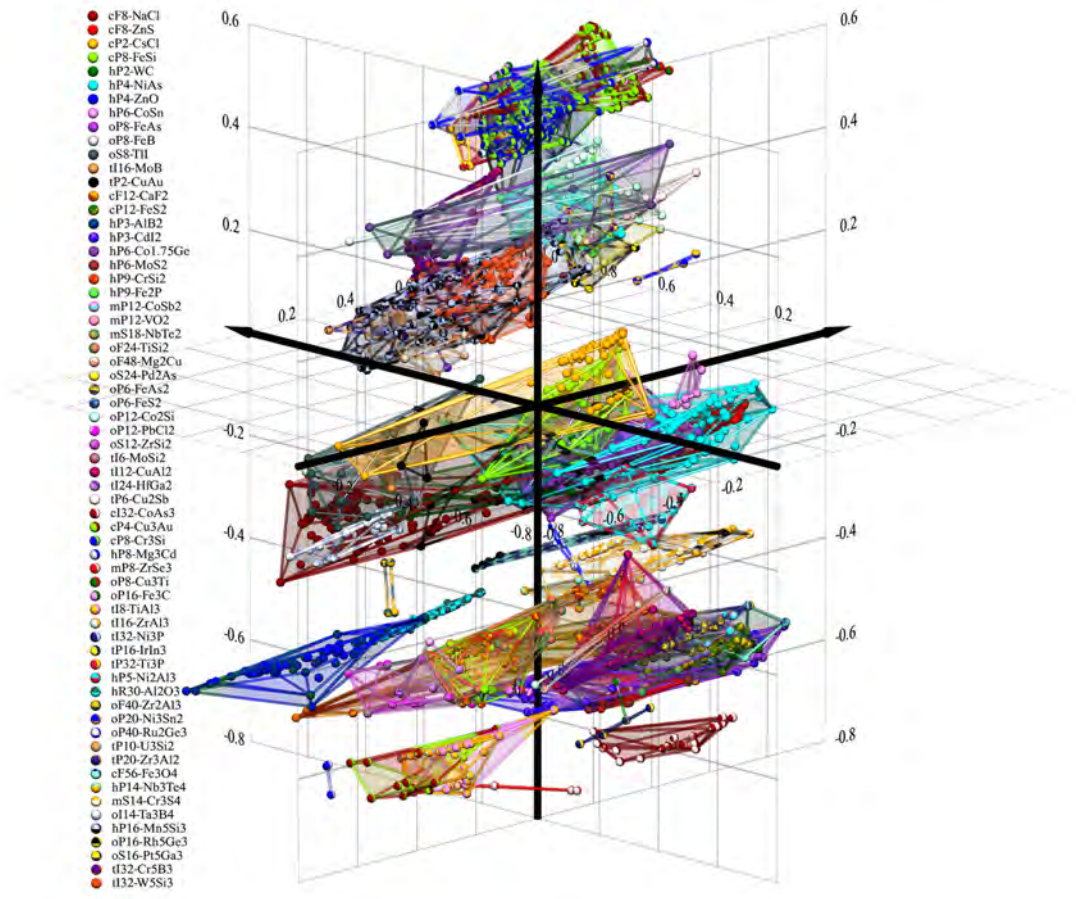


Fig. 4.9: Structure map for sp-d-valent compounds as derived systematically on the basis of crystallographic databases (Arthur Bialon).

Dr. Arthur Bialon derives structure maps for compound systems from crystallographic databases. In contrast to previous works, the approach taken is unbiased and relies on the automated identification of order parameters from large sets of combinations of atomic properties with functions that relate the elements to compounds. The resulting structure map (*Fig. 4.9*) allows us to predict the crystal structure of sp-d-valent systems with confidence values that are comparable to DFT calculations. This scheme allows for an instantaneous crystal-structure prediction and thereby reduces the time-to-solution drastically as compared to DFT calculations. The same procedure is currently applied to d-d-valent systems.

Alvin Ladines (PhD student of the IMPRS graduate-school SurMat) investigates the formation of complex intermetallic phases in Fe-based binary systems. This involves high-throughput DFT calculations as well as the development of analytic BOPs for TCP phases in the Fe-Nb system phases. The DFT calculations could, e.g., demonstrate that the relative structural stability of the Laves Phase C14, C15 and C36 is altered by external pressure (*Fig. 4.10*).

Dr. Jörg Koßmann compares Ni-based and Co-based single-crystal superalloys by means of electronic structure and atomic size using both high-throughput DFT and empirical structure maps. The chemical disorder in the Co-based systems is treated with cluster-expansions and special quasi-random structures (*Fig. 4.11*) The DFT results are further used in a joint effort with Dr. Mauro Palumbo, Dr. Suzana Fries, and Prof. Ingo Steinbach in order to explore routes for up-scaling in temperature by including entropy contributions to phase stability.

Ning Wang (PhD student funded by the China Research Council) started with modelling defects in II-VI semiconductors using bond-order potentials at ICAMS in 2014. The focus is currently on assessing the existing BOPs for the Cd-Zn-Te system that is used in X-ray detectors and solar cells.

Dr. Miroslav Čák investigates the melting behaviour and mechanical properties of refractory metals. He furthermore applies existing BOPs for Fe and Fe-C to the interaction of dislocations in Fe with vacancies and grain boundaries.

Sebastian Schreiber extends the functionality of the BOP simulation package and applies Fe and Fe-C BOPs in large-scale simulations of dislocation movement. In collaboration with Dr. Karthikeyan Chockalingam, Dr. Rebecca Janisch and Prof. Alexander Hartmaier, these BOP simulations are directly linked to continuum-scale simulations for dislocations in iron.

Jan Jenke started his PhD thesis in 2014 and develops systematic approaches for the parameterization of bond-order potentials. The target system Fe-Si shows the full complexity of interatomic bonding with transitions between metallic/covalent, metal/semiconductor and d-valent/sp-valent bonding.

The scalability of the parallel BOP simulations beyond million-atom systems was achieved in a joint effort with Dr. Carlos Teijero Barjos and Prof. Godehard Sutmann from the HPC group. This development was critical to reduce the required RAM per code in parallel calculations of large systems.

External collaborations include Dr. Fritz Körmann, Dr. Tilmann Hickel and Prof. Jörg Neugebauer (MPIE Düsseldorf), Dr. Matous Mrovec (Fraunhofer IWM Freiburg), Dr. Sascha Maisel and Prof. Stefan Müller (TU Hamburg), Prof. Vaclav Vitek (University of Pennsylvania, USA) and Prof. David Pettifor (University of Oxford, UK).

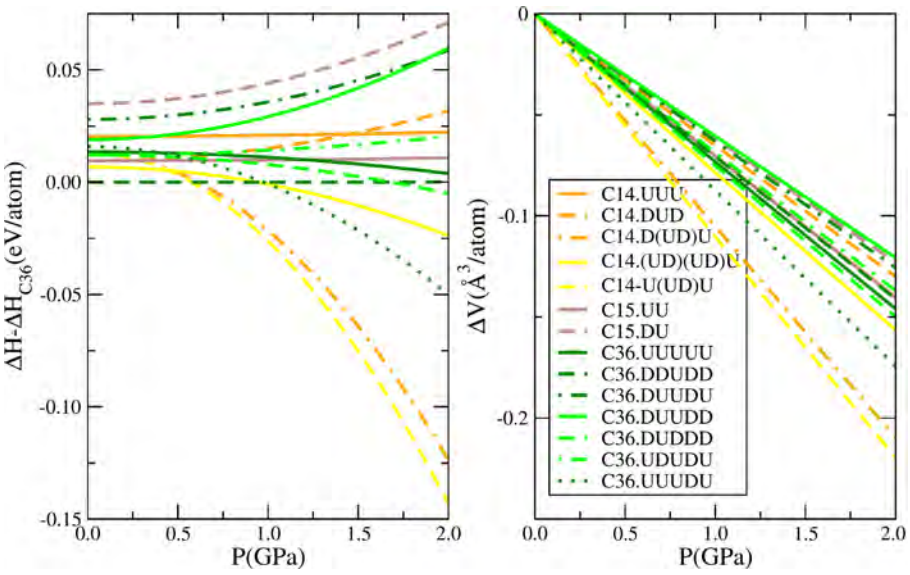


Fig. 4.10: Influence of hydrostatic pressure on the structural stability of Fe_2Nb Laves phase with different magnetic configurations as obtained from DFT (Alvin Ladines).

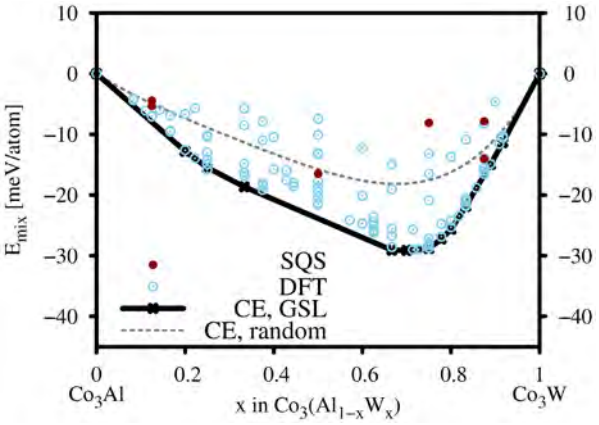


Fig. 4.11: Mixing energy in L12-Co_3 (Al,W) computed by DFT with chemical disorder modelled by cluster-expansion (CE) and special quasi-random structures (SQS) (Jörg Koßmann).

AMS

4.3 Atomistic Simulations of the Kinetics of Phase Transformations

Group leader:
Dr. Jutta Rogal

Group members:
Dr. Grisell Díaz Leines
Dr. Ari Harjunmaa
Dr. Thomas Schablitzki
Dr. Sergej Schuwalow
Dr. Daniel Şopu
Tanmoy Chakraborty
Martin Staadt

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

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

A key aspect in dynamical simulations on an atomistic level is the accurate evaluation of energies and forces within the system. System sizes that are required to treat structures containing extended defects are often too demanding for first-principles calculations, whereas simple interatomic potentials are not accurate and transferable enough to account for the diverse local environments in these structures. To allow for reliable energetics in large systems, a systematic development of tight-binding models and bond-order potentials is carried out within the AMS research groups of Dr. Madsen and Dr. Hammerschmidt, which could then also enter the dynamical simulations performed within Dr. Rogal's group.

Furthermore, electronic structure calculations performed within the AMS department and the Advanced Study Group 'Modelling' provide input for dynamical simulations. One of the key results of the kinetic simulations on the atomistic level is the extraction of parameters required in mesoscale models. These parameters provide a direct link to mesoscale and macroscopic models developed in the departments STKS and MMM and to experiments in the Advanced Study Group 'Input Data and Validation' led by Prof. Eggeler.

In 2014 Dr. Rogal's research group comprised the following projects:

Dr. Thomas Schablitzki successfully finished his doctoral studies in June 2014 with his work on the formation of TCP phases in FeCr, for which he developed a structure analysis method based on topological fingerprints. The topological fingerprints can also be used to characterise and identify atomistic processes taking place during the phase trans-

formation. The kinetics of the phase transformations were investigated by using the adaptive kinetic Monte Carlo (AKMC) approach and the transformation mechanisms were further characterised by a correlation analysis of the dynamical trajectories. Dr. Schablitzki has continued his work in the group as a postdoctoral fellow. He has started a new project on the calculation of temperature programmed desorption (TPD) spectra of hydrogen in iron, based on KMC simulations. Within the KMC simulations, diffusion as well as desorption processes are explicitly treated allowing for the interpretation of the experimentally measured spectra. The overall complex peak structure in the TPD spectra can be decomposed into contributions from hydrogen molecules that were trapped at different defect sites such as grain boundaries, substitutional defects or vacancies. This project is carried out in collaboration with the MPIE, Düsseldorf, and ThyssenKrupp Steel Europe.

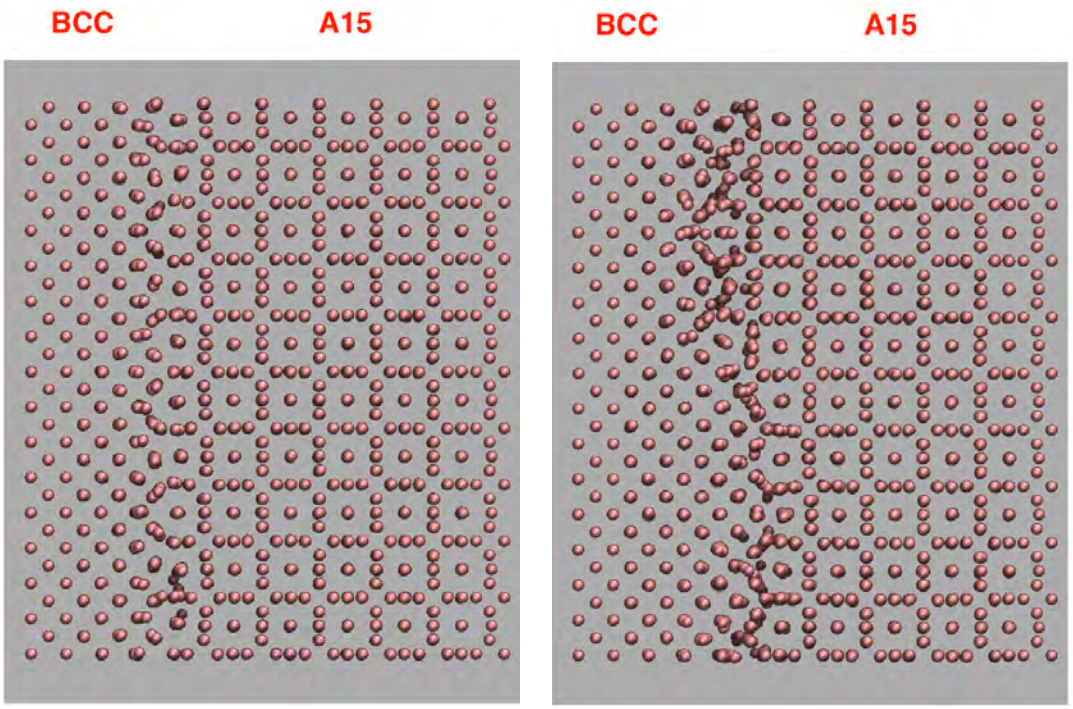


Fig. 4.12: Snapshots from a molecular dynamics simulation of the phase transformation from A15 to BCC in molybdenum. Initial configuration (left) and during the simulation, where a step nucleation and a growth mechanism are observed (right).

Dr. Ari Harjunmaa, who joined the group from March 2012 to May 2014, was working on long time-scale atomistic simulations of solid-solid phase transformations in molybdenum. He used the AKMC approach as well as molecular dynamics simulations to investigate atomistic processes at the interface between the body-centred cubic and TCP A15 phases, and to follow the migration of the interface. From the simulations, an effective layer transformation time, which showed an Arrhenius type behaviour, could be extracted. The resulting apparent activation barrier was, however, not directly associated with a particular atomistic process at the interface but rather with the overall topology of the potential energy surface during the transformation. Simulations in larger cells revealed that the transformation proceeds via step nucleation and growth mechanism at the interface (*Fig. 4.12*).

Dr. Daniel Şopu was a postdoctoral researcher in the group from April 2012 to May 2014. He employed transition path sampling (TPS) techniques to investigate solid-liquid phase transformations. A particular focus was put on the analysis of the path ensemble with respect to transformation mechanisms, interfacial properties, and the identification of suitable reaction coordinates. The methodological work for a Lennard-Jones system was complemented by TPS simulations to determine the solid-liquid interfacial free energy in FCC aluminium. Due to the rather high computational cost of these simulations, an embedded atom method (EAM) potential was used for aluminium. In collaboration with Dr. Xueyong Pang and Dr. Rebecca Janisch from the Department MMM, a quantitative comparison of the TPS and metadynamics methods was performed. Both methods were in good agreement and also compared well to previously reported values in literature.

Within the DFG collaborative research centre SFB-TR103, Dr. Sergej Schuwalow started his research project in July 2012. He is investigating the influence of central d-band elements in Ni-based superalloys with a focus on the mobility and segregation behaviour using both density-functional theory calculations and kinetic Monte Carlo models.

Tanmoy Chakraborty started his doctoral thesis in June 2013 and is working on an atomistic description of martensitic transformations in the Ti-Ta system, a new material exhibiting a shape memory effect at elevated temperature above 373K. His project is part of the DFG research unit FOR1766. Using the solid-state nudged elastic band (SSNEB) method together with density functional theory (DFT) calculations, he determined the minimum energy paths for the transformation between the three involved phases β → (α″,ω) as a function of composition (*Fig. 4.13*). Furthermore, to a first approximation, the change in relative stability of the different phases as a function of Ta content could be related to the change in the martensitic start temperature. As a third important aspect, the dynamical stability of the phases at T=0K was evaluated by calculating elastic constants and phonon spectra. The phonon spectra showed a clear dependence of the dynamical stability on the composition, and indicated the importance of extending the current approach to finite temperature.

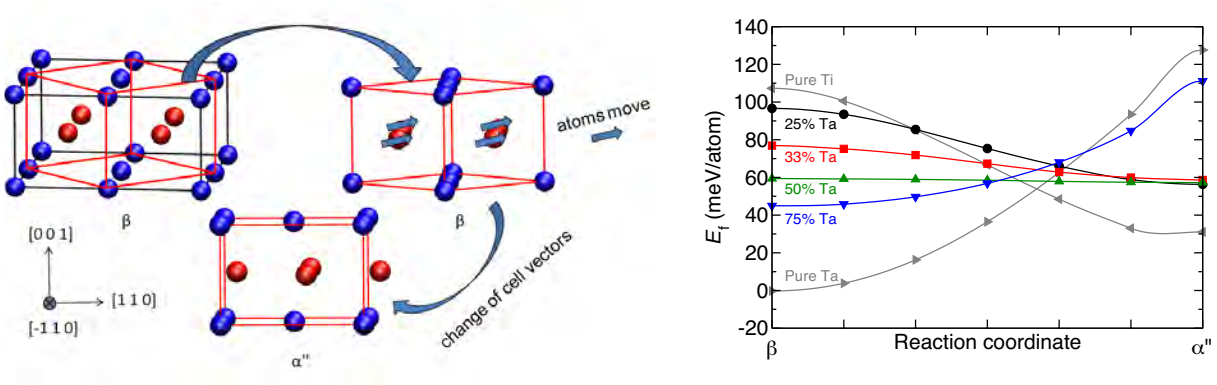


Fig. 4.13: Orientation relationship between the β and α″ phase in titanium-tantalum (left). Minimum energy paths of the β → α″ transformation as a function of composition (right).

Martin Staadt began his doctoral studies in June 2014 within the International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS-SurMat). His project focuses on the investigation of interfaces in iron, in particular between austenite and ferrite. A key aspect in his work is the determination of free energies by using thermodynamic integration on the basis of bond-order potentials. Due to the complex magnetism in the iron system, it is important to explicitly treat the electronic structure and include the magnetic contributions to the free energy.

Dr. Grisell Díaz Leines joined the group as a postdoctoral fellow in June 2014. She has received a fellowship from the Consejo Nacional de Ciencia y Tecnologia science foundation. Within her project, she uses TPS sampling to investigate nucleation during solidification in nickel (*Fig. 4.14*). The path ensemble provides information about the free energy of the nucleation process and thus information about the nucleation barrier as well as the nucleation mechanism. From the transition state ensemble, the size and shape of the critical nuclei as a function of undercooling can be established. Furthermore, the simulations allow for a direct comparison of homogeneous and heterogeneous nucleation at defects and the investigation of the effect of size and shape of nucleation seeds. The atomistic simulations provide an assessment of classical nucleation theory and can also be used to derive input parameters for phase-field models of solidification.

Collaborations outside ICAMS have been established with the MML at the University of Oxford in the area of TCP phases and tight-binding models/bond-order potentials. In the area of Markov state models, the collaboration with Prof. Graeme Henkelman, University of Texas at Austin, has been continued. Approaches to free energy calculations are tested and developed in collaboration with Prof. Mike Finnis, Imperial College, London, and Prof. Mark Asta, University of California, Berkeley. Close collaborations, particularly with experimental groups, are intensified within the DFG collaborative research centre SFB-TR103 and the DFG research unit FOR1766.

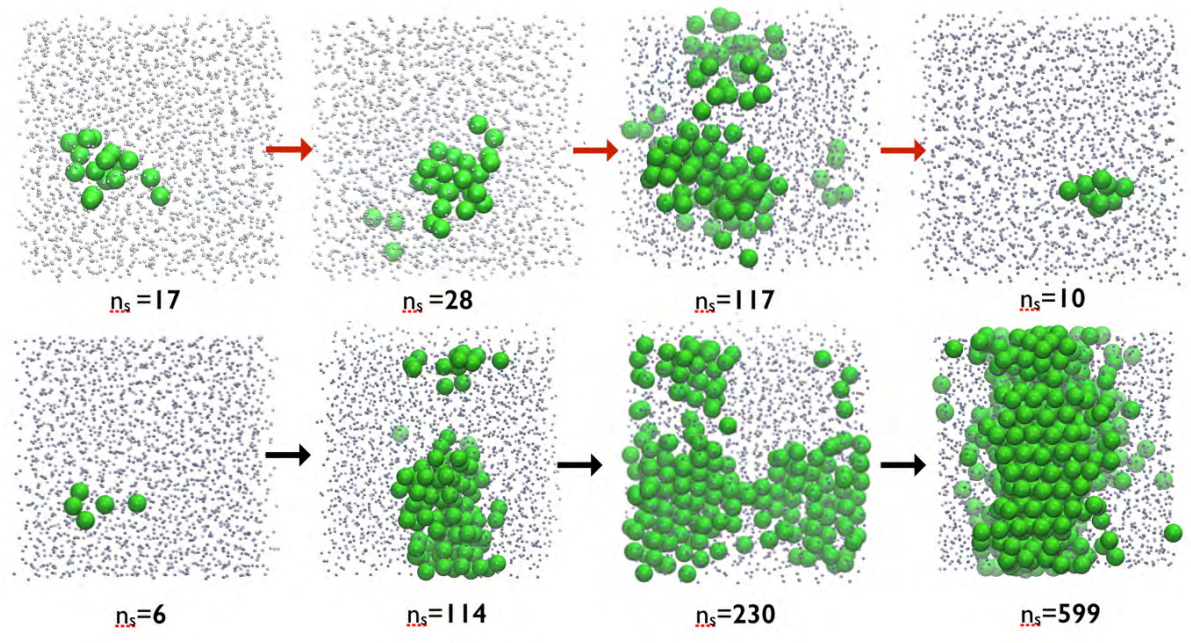


Fig. 4.14: Snapshots from a transition path sampling simulation of the nucleation during solidification in nickel at 25% undercooling. The value of n_s indicates the size of the largest cluster. The trajectory shows the formation of a solid cluster up to n_s=117 that is again dissolved (top). The solidification proceeds and the nucleation barrier is overcome, resulting in the formation of a FCC solid (bottom).

Department Scale Bridging Thermodynamic and Kinetic Simulation STKS

5. Department Scale Bridging Thermodynamic and Kinetic Simulation

Prof. Dr. Ingo Steinbach

Research

The department's research is focused on bridging the atomistic nature of condensed matter to the macroscopic scale of materials properties. Methods applied are CALPHAD thermodynamics of multicomponent alloys, phase-field kinetics of microstructure evolution, Lattice Boltzmann fluid dynamics, and molecular dynamics simulations of soft-matter phenomena. We use commercial software as well as self-developed software tools we share with others according to an open, general public license philosophy.

Materials and mechanisms

We work on a wide spectrum of material classes, from pure metals and technical alloys, such as steels and Ni-based superalloys, to ceramics and polymers. On the mesoscopic scale, the different mechanisms of microstructural evolution processes are more important for our research than the specific class of a material. Based on the minimisation of the total free energy of the material (modified by surfaces and defect structures), kinetics of microstructure evolution are predicted, including the transport of solute and energy, as well as phase transformations. Phenomena studied include coarsening, wetting and dewetting, diffusion-controlled and displacive phase transformations, precipitation and ordering as well as deformation and flow in crystalline and amorphous materials.

2014 news and highlights

In 2014 the Third International Symposium on Phase-Field Modelling (PFM14) took place at Pennsylvania State University, chaired by both Long-Quing Chen and Prof. Ingo Steinbach and was visited by more than 100 participants. The PFM series started in 1999 as a decennial event and took place at Rolduc Abbey, The Netherlands. The second meeting was held in 2009. Due to the rapid growth of the field, it has been decided to halve the period and to switch the location to varying sites. The forthcoming symposium is announced to take place at the Ruhr-Universität Bochum, Germany, in 2019.

Fig. 5.1: Group photo of PFM14 participants. Bottom left: Yunzhi Wang, designated co-chairman of PFM19, Long-Quing Chen, and Prof. Ingo Steinbach, Chairmen of PFM14.

Fig. 5.2: Group photo of STKS members, January 2015.

The new DFG priority program SPP 1713 "Strong coupling of thermo-chemical and thermo-mechanical states in applied materials", started its active period in 2014. 16 single projects are funded and grouped into four areas. The first plenary meeting was held at the Ruhr-Universität Bochum. The priority program brings together researchers from all over Germany, including metallurgists and polymer scientists.

22 papers have been published by STKS members in refereed journals in 2014, among them the article "Multiple reentrant glass transitions in confined hard-sphere glasses" by S. Mandal, S. Lang, M. Gross, M. Oettel, D. Raabe, T. Franosch and F. Varnik, published in Nature Communications. Additionally, eight master theses and two PhD theses were successfully defended during the year.

STKS

5.1 CALPHAD Thermodynamics

Group leader:
Dr. Suzana G. Fries

Group members:
Dr. Mauro Palumbo
Dr. Abed Breidi
Irina Roslyakova
Farnoosh Falsafi

Fig. 5.3: The CALPHAD Thermodynamics group; from left to right: A. Breidi, A. Samimi, S. Tumminello (guest from National University of Comahue), F. Falsafi, S. G. Fries, T. Davey (guest from Inperial College, London), M. Palumbo.

The goal of the group is to incorporate first-principles calculated quantities into the thermodynamic modelling of Gibbs energies of stable and metastable phases following the CALPHAD method, in order to provide robust and sustainable multiphase thermodynamic data for microstructure simulations. The methodology to achieve this goal is developed within the Sapiens project.

The use of density functional theory (DFT) to calculate electronic and vibrational contributions to the heat capacity opens the possibility for better understanding and, as a consequence, better controlling of the evolution of those contributions with temperature. This provides a physical insight into the pure mathematical parameters used till now in the CALPHAD Gibbs energies temperature dependence. For the composition dependence of Gibbs energies describing ordered phases, we map the configuration of several crystal structures and calculate enthalpies of formation at zero K using DFT in collaboration with the Department AMS. We assume a Bragg-Williams approximation for configuration entropy as the main contribution to the entropy. For the disordered phases we have given preference to the EMPO-CPA method, but SQS and the cluster expansion method are also under investigation. The application of our Gibbs energies functions database for multicomponent, multiphase materials requires a realistic description of experimentally observable quantities. In order to fulfil this requirement, we construct an extensive experimental database which is used for training the physical parameter of the models. We add excess quantities when necessary, but with our method they are usually a small correction to the well-controlled physical quantities.

In 2014 we continued the strategy of inviting senior scientists as well as students in order to consolidate and expand our method. The main routes of development of the group were as follows:

a. Experimental databases: We continued to collect experimental data directly from publications. Values were stored in tables when available or digitized. We extended this data acquisition to binaries systems relevant to Co- and Ni-based alloys. The organisation of these data is done in close collaboration with the MGI (Material Genome Initiative), a project coordinated by the National Institute of Standards and Technology, NIST, represented by Eric Lass, Carelyn Campbell, and Ursula Kattner, who visited ICAMS in 2014, and is presently focused on Co-based alloys.

b. Software development: Open CALPHAD (OC) code was released in its version 2 (www.opencalphad.org). The main developer of the code, B. Sundman, who visited us within the scope of the Humboldt Award and who has recently been working in cooperation with the Phase-Field-Simulations group, made possible the coupling of the OC with the OP (OpenPhase) code. A generic interface TQ was created. Updates can be found at the project's website. The scope of the OC initiative description was accepted for publication in Integrating Materials and Manufacturing Innovation (IMMI).

c. Extension of first-principles calculations: First-principles calculations of elements relevant to Ni- and Co-based superalloys and of those intermetallics (TCP phases) which are most common in these alloys were extended. These calculations were done together with the Department AMS (Jörg Koßmann and Thomas Hammerschmidt) and members of the ASG Modelling (Tilmann Hickel and Fritz Körmann). We now have the complete first-principles formation energies for all phases in the Al-Co, Al-W and Co-W, Co-Ti, Ni-Al binaries as well as Al-Co-W and Co-Ti-W ternary systems and their description in the compound energy formalism based only on the theoretical results. We coordinate the subsequent optimisation methods taking into account experimental data from Gabriele Cacciamani (Co-Ti), Nathalie Dupin, Silvana Tumminello (Ni-Al), Ursula Kattner (Co-Ta) and Andreas Markström (Co-W). All these researchers have access to the first-principle configuration enthalpies, and the assessments are being done in a cooperative mode. We also envisage including elastic constant tensors in a consistent way in the databases (TDB files) in cooperation with ThermoCalc Software AB and KTH Stockholm.

d. We initiated a co-operation on B-C-Hf-Zr quaternary systems with Mike Finnis and his PhD student Theresa Davey. In this work, a standard CALPHAD database is created, based on previously known information. Some special properties of first-principles (e.g., heat-capacities for HfC and ZrC) are also being studied and developed in their laboratory. The results will be compared to the same quantities as calculated from the CALPHAD database.

During 2014 we hosted visiting students of M. Selleby, Stockholm and of M. Finnis, London. The collaboration with J. Johansson, Lund, continued, and a CALPHAD method overview course was organised at Lund University in April, coordinated by M. Ghasemi. Since October, S. Tumminello, a PhD candidate from Argentina and granted by DAAD, has been visiting us.

Suzana G. Fries and Rebecca Janisch from MMM organised the "Prediction and Characterization of Material Microstructures by Simulation and Experiment" school at Weeze in September. The School had lecturers from the departments STKS, MMM and AMS as well lecturers from KTH Stockholm. It included students from both research centres and industrial partners as participants.

Fig. 5.4: The participants of the ICAMS Hero-M School at Weeze.

Progress in the modelling of Co-based superalloys

We continued the Sapiens project for Co alloys and have now the binary systems Co-Al, Co-W, Al-W, Al-Ni, and Co-Ti. All descriptions have been obtained from first principles enthalpy calculations for stable and metastable phases provided by the Department AMS. The temperature dependence is obtained by the Bragg-Williams approximation (also parameter free as the configuration entropy is obtained from the first-principle calculated lattice-site occupancy multiplicity.

The inclusion of the so-called TCP phases without a priori selection in all the calculations, results in a very promising phase/composition range stability prediction. The comparison to the equilibrium experimental phase diagrams (well captured by the present CALPHAD description available in literature) is presented for some selected systems. Also metastable order/disorder FCC-based phase diagrams are presented.

Work is now being done to add the unaries database done previously where phonons and electronic contribution were taken into account.

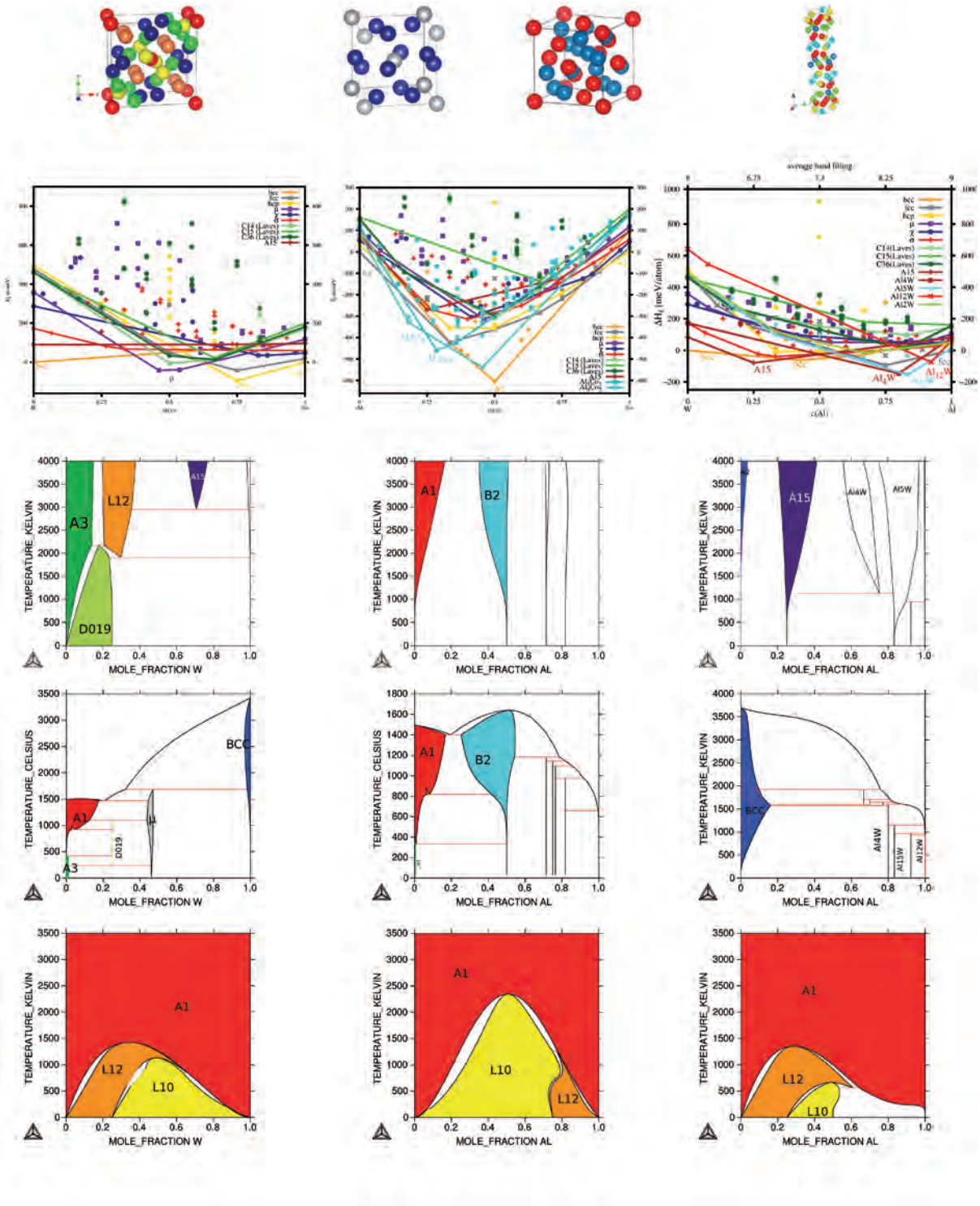


Fig. 5.5: The first row of diagrams shows the enthalpies of formation calculated with DFT for several crystal structures for permutations of two selected atoms (Co and W, Co and Al and Al, W) in all the crystallographic sites of the selected crystal structures. The second row presents the phase diagrams calculated using exclusively the first-principles data of the first row respectively. The third row shows the CALPHAD phase diagrams as presented in the TCNI6 database, which should capture the experimental evidences the modelling is based on and the last row shows the metastable FCC-based phase diagrams for the three systems.

STKS

5.2 Phase-field simulation of microstructures

Group leader:
Dr. Oleg Shchyglo

Group members:
Adam Andreas Gießmann
Mohan Kumar Rajendran
Efim Borukhovich
Matthias Stratmann
Alexander Monas
Johannes Görler
Guanxing Du

Introduction

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

Research highlights

Development of the OpenPhase phase-field simulation library

During the year 2014 our open source project OpenPhase (*www.openphase.de*) has undergone several optimisations and a significant increase in simulation possibilities. The recent version of the library allows simulating systems that consist of a high number of grains of different thermodynamic phases, including stoichiometric ones. At present, all simulations in our group are performed by using the OpenPhase library. These include simulations of grain growth, peritectic and eutectic reactions in carbon steel, rafting in superalloys, as well as eutectic solidification with and without the forced and gravitational convection in the melt. The latter is carried out in collaboration with the 'Theory and simulation of complex fluids' group that additionally provided the Lattice Boltzmann fluid-flow solver for the OpenPhase project.

Eutectic solidification of Mg-Al alloy - Alexander Monas

Magnesium alloys are among the most promising structural materials for lightweight applications, due to their low density compared to aluminium and steel. The mechanical properties of Mg-Al alloys are primarily determined by their microstructure which consists of two main phases - the Mg-rich hexagonal close-packed (HCP) α-phase and the near stoichiometric $Mg_{17}Al_{12}$ β-phase as well as further minor secondary phases due to third alloying elements. The addition of Al in small concentrations has a positive effect on the corrosion properties of the Mg-Al alloys mainly due to the formation of a percolating β-phase network which is less electrochemically active com-

pared to the α-phase. Experiments reveal that the formation of a closed shell of β-phase, which prevents α-phase dendrites from building networks, is a good strategy to significantly increase the corrosion resistance of cast Mg-Al alloys.

Simulations are performed on two different scales. Although the primary solidification in three-dimensional domains can be investigated in order to reveal the effect of the cooling rate on the nucleation density of α-phase dendrites, it is computationally demanding to study the entire solidification process in 3D over the temperature range of more than 200 K even with high cooling rates.

In contrast, it is possible to investigate the entire solidification process in 2D simulations starting from the primary α-phase dendritic solidification and continuing with the eutectic

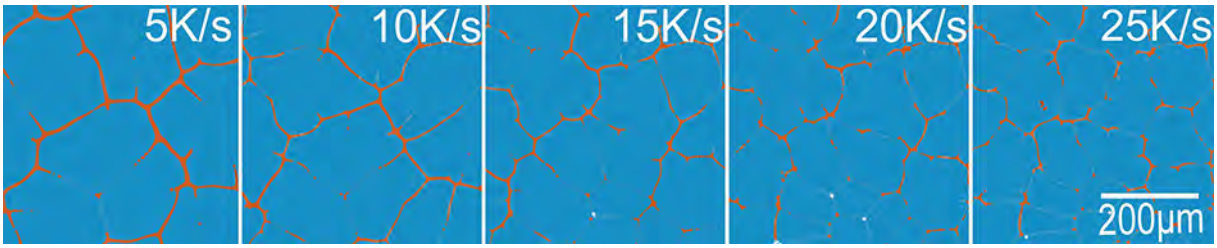


Fig. 5.6: 2D simulated microstructures of Mg-Al alloys solidified at different cooling rates. The primary α-phase is shown in blue, the secondary β-phase in orange.

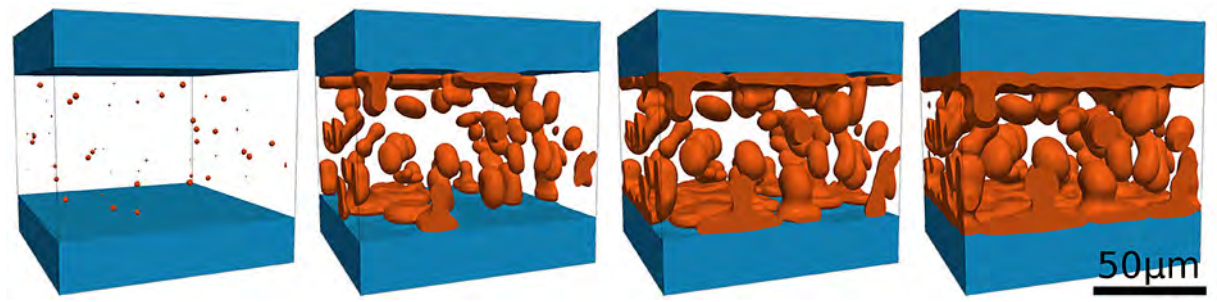


Fig. 5.7: Zoomed-in region of the residual eutectic melt channel between two α-phase dendrites (blue) at different time-steps.

solidification of the secondary β-phase upon cooling below the eutectic point. The results are shown in *Fig. 5.6*.

A clear trend of increasing α-phase grain density with increasing cooling rate can be observed, which is in agreement with experimental observations. This behaviour is achieved naturally by the implementation of a free growth model proposed by Greer et al. which allows reproducing the re-coalescence effect responsible for the increased nucleation density at higher cooling rates.

In order to investigate eutectic growth in detail, we zoom into the channel between two primary dendrites upon reaching the eutectic temperature. Here, we select the scale of the simulations by a factor of 5 finer than the scale of primary α-phase dendritic solidification simulations. The heat extraction rate is assumed constant, which relates to an applied cooling rate (neglecting release of latent heat). The simulations of divorced eutectic growth start from a concentration profile taken around the melt channel of a 2D simulation of primary α-phase growth.

As can be seen in *Fig. 5.7*, the growth of the secondary β-phase shows a tendency towards the formation of a closed shell around the α-phase dendrites leading to the divorced eutectic solidification scenario. The formation of the closed shell β-phase formation is responsible for increasing the corrosion-resistance of Mg-Al alloys. The good agreement of the simulation results with experimental observations allows using the proposed simulation method for a computationally assisted design of corrosion-resistant Mg-alloys.

γ – γ'-microstructure stability analysis in Ni-based superalloys - Johannes Görler

Nickel-based superalloys are exceptionally well suited for applications demanding high temperature resistance as well as excellent mechanical properties. The microstructure consisting of cuboidal γ-phase precipitates embedded in a γ-phase matrix is one of the main factors in obtaining these beneficial properties. Therefore it is important to investigate possible changes to the desired microstructure that could occur under service conditions. Here, the microstructure evolution during a long term aging treatment is studied by means of phase-field simulation. Additionally, the mechanism stabilising the desired microstructure is investigated.

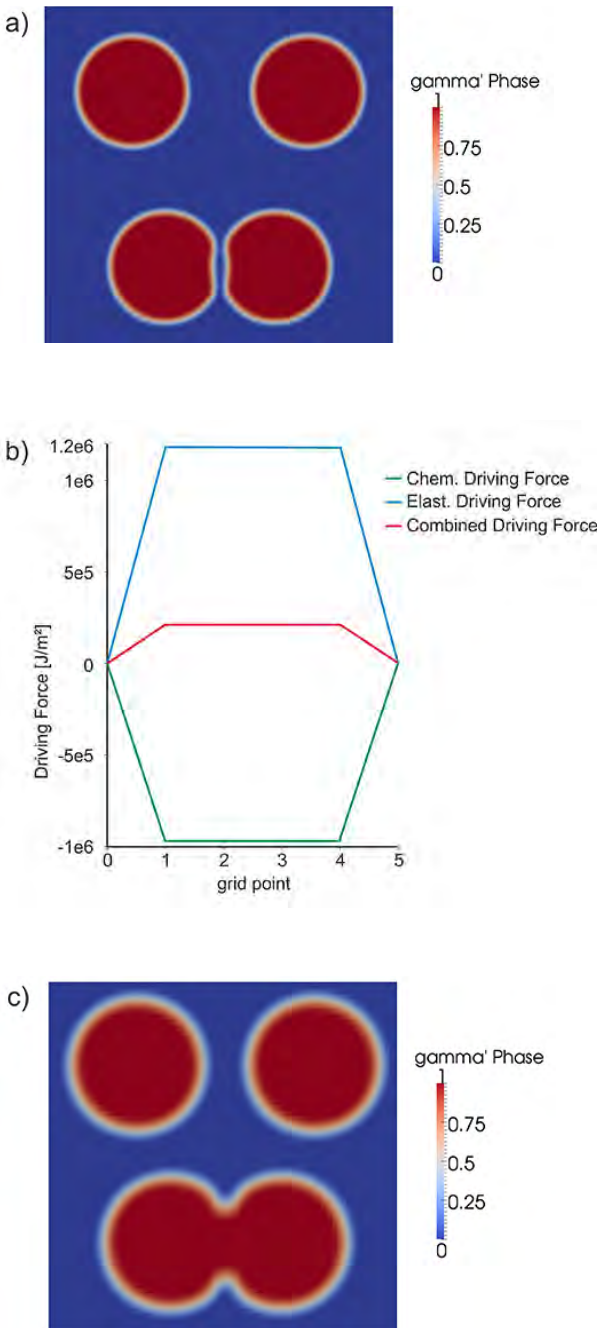


Fig. 5.8: Stabilization of the γ channel: a) grid spacing 2.5 nm b) balance of chemical and elastic driving force in the interface c) grid spacing 5 nm.

The γ/γ' microstructure usually consists of more than 60 vol. % of the precipitating γ-phase. Therefore, the γ matrix is the minority phase. A topological inversion of the microstructure, i.e., the precipitating phase topologically becoming the matrix phase, would be energetically beneficial because of the lower interface energy contribution. However, the microstructure is very stable. Therefore, a mechanism has to be active that prevents the coalescence

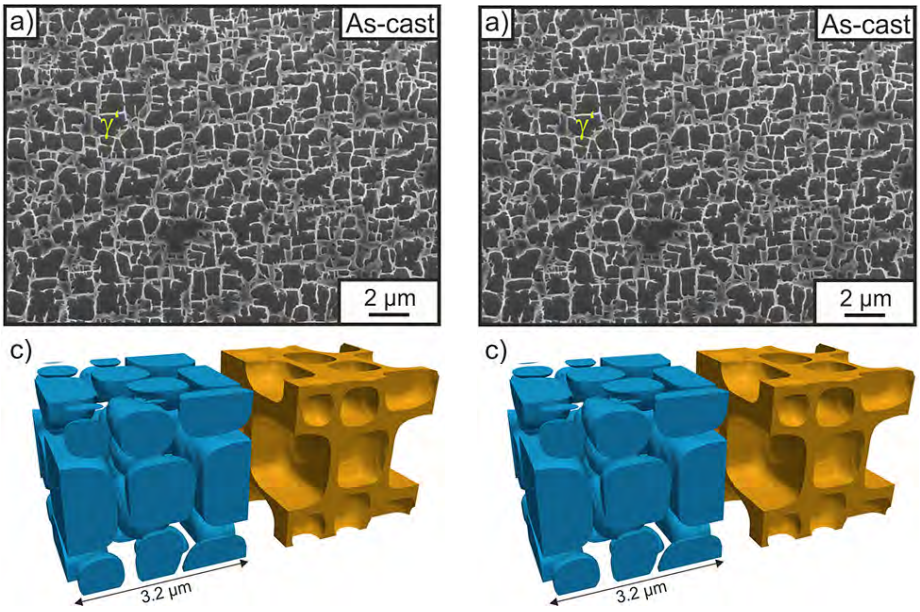


Fig. 5.9: Long term aging experiment and phase-field simulation: a) As-cast state b) 250 h aged at 1100˚C c) simulated initial microstructure and d) simulated aged microstructure.

of the γ precipitates from coalescing. The proposed mechanism is that the elastic energy for a decreasing γ channel width between two γ precipitates increases significantly. Thereby, an equilibrium state between a chemical driving force and an elastic driving force is reached and the coalescence of γ particles is prevented. This is tested in a two-dimensional phase-field simulation with four precipitates of different sizes. *Fig. 5.8 (a)* shows the repulsive behaviour of the two γ'-precipitates, while in *Fig. 5.8 (b)* the balance of the elastic and chemical driving force resulting in the stabilisation of the γ-channel is shown. The simulation of the stabilising effect strongly depends on resolution. Fig. *5.8* (c) shows the same simulation setup as in *Fig. 5.8 (a)*, but with the grid spacing doubled. Here the stabilisation does not occur because both of the γ/γ' interfaces overlap before the balance of driving forces is reached. Once the interfaces overlap, the system minimises the interface energy by merging the interfaces and therefore removing the γ-channel.

During long-term aging of Ni-based superalloys, dislocation networks surround the γ-precipitates. The dislocations arrange in such a way that the misfit strain between the γ- and γ'-phase is significantly reduced. Thereby, the mechanism stabilizing the γ/γ'-microstructure is gradually removed, and γ'-precipitates are able to coalesce. Experimental and simulation results are shown in *Fig. 5.9* with the initial microstructures (a) and (c) and the aged ones (b) and (d).

Martensite microstructure modelling - Guanxing Du

Martensitic transformation is a first-order diffusionless solid state phase transformation that can happen in most heat-treatable commercial carbon steels. When the austenite phase with a face-centred cubic structure is rapidly quenched to a certain low temperature, a displacive transformation forms a new highly strained phase with a body-centred cubic or a body-centred tetragonal structure. As the mechanical properties of martensitic steels are greatly affected by the microstructure, an ample amount of investigation on the morphology and crystallography of martensite has been done over the past fifty years. Furthermore, a lot of numerical simulations of martensitic transformation by using various theories and methods are also developed to characterise the microstructure as well as the growth behaviour of martensite.

In our work, we are aiming to predict the initial microstructure of tempered martensite by using the phase-field method. This will be the basis for a scale-bridging model of the microstructure evolution and the related mechanical properties research.

For the low carbon steel that is mainly investigated in this work, the microstructure is formed by transformation of the original austenite into packets (the group of martensite laths with the same habit plane) and each packet is further

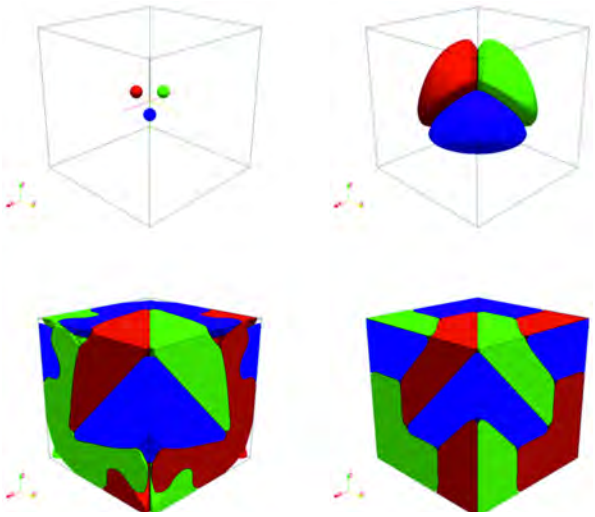


Fig. 5.10: Evolution of three variant martensite.

subdivided into blocks (the group of lath with the same orientation). Although the orientation of each martensite lath is scattered around some ideal values, there are mainly four orientation relationships - ORs - to describe the lath martensite: Bain OR, Nishiyama-Wassermann (N-W) OR, Kurdjumov-Sachs (K-S) OR and Greninger-Troiano (G-T) OR.

According to the nature of martensitic transformation, the formation of martensite patterns is associated with the internal strain accommodation between different martensite variants which together with the latent heat release dominate the transformation kinetics. The far goal of this project is to study the martensite microstructure formation including its autocatalytic nucleation by using the phase-field method coupled to the microelasticity and the crystal plasticity model.

We start our simulation with the small strain martensite (0.5% ~ 1%), assuming a purely elastic condition. Three different Bain strain variants of tetragonal martensite are placed in the middle of the austenite grain and let grow as shown in *Fig. 5.10*.

In the next step, the martensite nucleation model is incorporated in order to investigate the autocatalytic nucleation of martensite. In this case, the simulation starts from a single variant of martensite in the austenite grain. Then, the nucleation events of other martensite variants are only determined by the elastic state and the critical nucleation energy at a given point. *Fig. 5.11* shows the martensite microstructure evolution including the autocatalytic nucleation in single prior austenite grain.

In the pure elastic simulation, the patterns of the martensite microstructure showed an ideal twin structure characteristic to Bain OR because the small deformation can be fully elastically relaxed. However, in real systems, due to the large lattice distortion of more than 13% between austenite and martensite, the anisotropic plastic relaxation as well as hardening in the matrix will significantly affect the growth of martensite forming lath and blocks. Therefore, incorporation of a crystal plasticity model is our next step in the 3D martensite formation modelling.

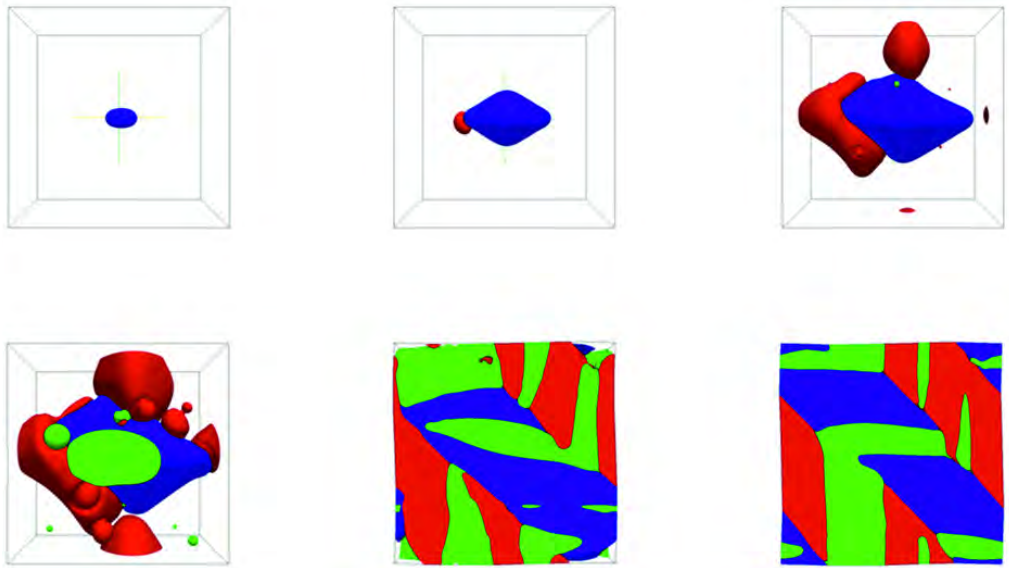


Fig. 5.11: Martensite growth with autocatalytic nucleation.

Large deformation modelling - Efim Borukhovich

As the natural extension of the phase-field model which uses purely elastic mechanical degrees of freedom that only allow simulations with small transformation strains, we incorporated the large deformation framework in order to study the transformations and material processing steps involving large strains.

During the last year the previously developed large deformation framework was extended by considering the grain orientation and its evolution during the deformation process. As an application example, a simulation of an anisotropic multigrain system was performed.

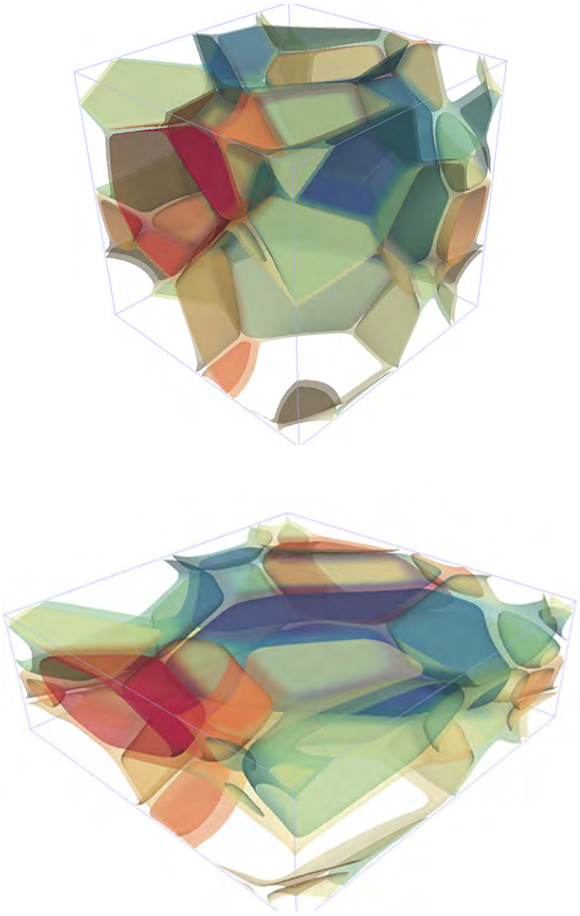


Fig. 5.12: Simulation result of the 50% thickness reduction of the multigrain system.

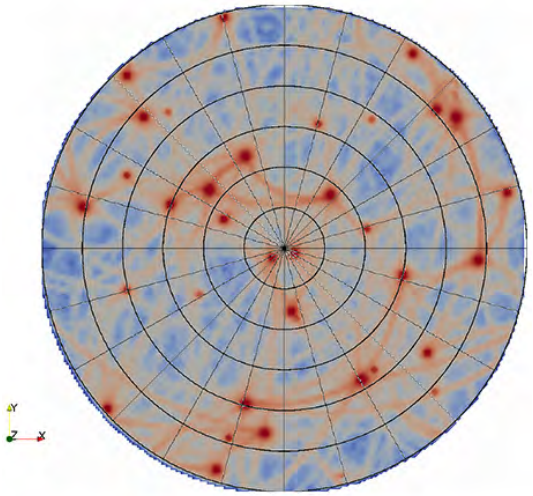


Fig. 5.13: (001) pole figure of the initial state.

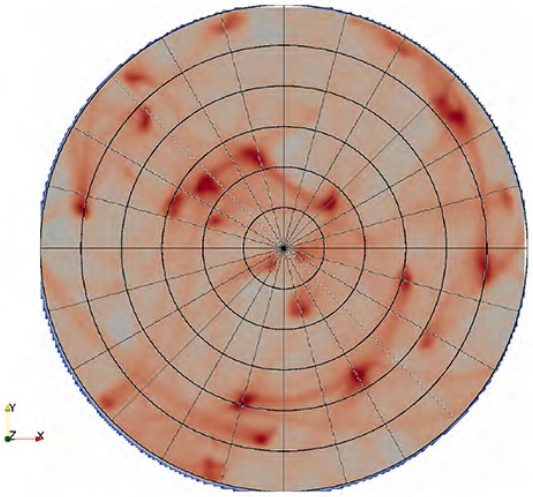


Fig. 5.14: (001) pole figure of the deformed state.

Since the global grain orientation as well as the local material point orientation present in the system continuously vary during the large deformation process, the orientation poles of the single grains are non-uniformly spread as shown in *Fig. 5.13* and *Fig. 5.14*.

The use of the large deformation model allows simulations of hot and cold rolling steel-making processes as well as the large strain martensitic transformations in steels, if the large deformation model is coupled to the crystal plasticity model, which is our next development step.

STKS

5.3 Theory and Simulation of Complex Fluids

Group leader:
Dr. habil. Fathollah Varnik

Group members:
Muhammad Reza Hassani
Suvendu Mandal
Nima Hamidi Siboni
Amol Subhedar

The research interest of the group is on transport phenomena and phase transformations in fluidic media. The focus of the group's work is two-fold. On the one hand, well-established numerical tools and theoretical approaches are used to uncover new phenomena such as the multiple reentrant glass transition in strongly confined fluids. On the other hand, innovative computational schemes are developed to allow the study of new types of problems in material science and engineering. An example of the latter case is the development of a hybrid phase-field Lattice Boltzmann code for phase transformation kinetics in the presence of transport by the flow.

In the year 2014 the complex fluids group consisted of five members. Muhammad Reza Hassani, who joined the group in October 2013, started his PhD studies on flow instability and shear banding in amorphous solids. A particular focus of this work has been on the role of spatial correlations, mediated by an elastic medium, in the plastic response and flow in these systems. As a senior member of the group, Suvendu Mandal succeeded in publishing his findings on the above mentioned multiple reentrant glass transition in Nature Communications. By the end of 2014 Suvendu completed and successfully (summa cum laude) defended his PhD thesis at the RWTH Aachen. Surya Narayana joined the group in June 2014 as a research student working on the bubble flow via Lattice Boltzmann simulations. Since then, he has been admitted to the Computational Engineering Master´s program at the Faculty of Mechanical Engineering and has continued his research in the group. The year 2014 provided the group with another 'summa cum laude' as Nima Hamidi Siboni defended his PhD thesis at the RWTH Aachen in November 2014. During the three years of his PhD studies, Nima investigated the physical relevance of the concept of effective temperature as a measure of mechanical noise in amorphous systems. As a major result, he demonstrated a close connection between mechanical noise and spatial correlations of plastic flow in amorphous solids. Amol Subhedar joined the group in April 2013 and has since been working on the implementation of a hybrid phase-field Lattice Boltzmann method to study the effect of flow on solidification and microstructure evolution. Thanks to his efforts and thanks to a close collaboration with Marvin Tegeler, a talented PhD student from the high performance computing (HPC) group (led by Godehard Sutmann), an efficient MPI-parallel version of the open-phase software, coupled to the lattice Boltzmann method, has been developed and tested successfully. We are now in the stage to tackle this demanding task with large-scale massively parallel simulations. In the following, a selection of the research highlights of the group will be presented.

It is well established that dynamic correlations grow in glass forming liquids as the glass transition is approached. The corresponding correlation length is, however, generally found to be limited to a few particle diameters. A dramatic change may occur if the glass is driven by an applied shear that forces structural rearrangements. Such external driving can lead to avalanche-like plastic response, mediated by a long range elastic field. This issue has been recently addressed for a hard sphere glass both via

computer simulations and experiments with a focus on direction-dependence of correlations and the crossover from the thermal regime of supercooled liquids to the athermal limit of strongly driven glasses. Qualitative agreement was found between simulations and experiments regarding both the behaviour of single particle fluctuations (found to be isotropic) and the anisotropy of their spatial correlations. The specific functional form of these correlations was, however, found to be different. While experimental data were best described by a power law decay – reminiscent of a self-similar behaviour – simulations suggested an exponential decay with a characteristic length of the order of a few particle diameters. We have addressed this issue via extensive simulations in two dimensions so that larger system sizes could be investigated. Results obtained from these simulations provide strong evidence that a reason for this discrepancy is the finite system size of previous three-dimensional simulations. Via event-driven finite-temperature simulations in 2D, we find that the exponential decay found for smaller sizes changes to an algebraic decay at larger L (*Fig. 5.15*).

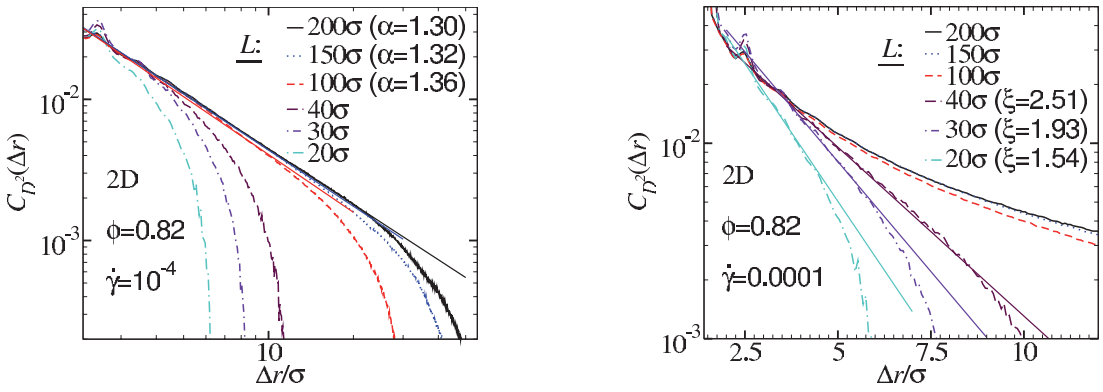


Fig. 5.15: Angle averaged correlation of plastic activity in two-dimensional simulations of hard disks for various system sizes in double-logarithmic (left) and semi-logarithmic (right) scale. The packing fraction is $\varphi = 0.82 > \varphi_g = 0.80$ (glassy state). The straight lines in the left panel are power-law fits, $(\Delta r)^{-a}$. This highlights the fact that correlations become of power-law type in the limit of large system size. In the right panel, on the other hand, they represent exponential fits, $\exp(-\Delta r/\xi)$. Apparently, correlations of plasticity deviate significantly from an exponential behaviour as the system size increases.

This is reminiscent of long range correlations close to a critical point. Indeed, the emergence of a long range power-law elastic field at the glass transition is believed to play a central role for the plastic response of amorphous solids. There is growing evidence that local plastic deformation at different points in the material influence one another via the accompanying elastic field. Within this picture, each local plastic event plays the role of an Eshelby inclusion in an isotropic and homogeneous elastic matrix. The long range stress field created by such an inclusion increases the probability for similar events in the surrounding medium, thereby giving rise to long range correlations of plasticity.

Another research topic the group is concerned with is the investigation of properties of strongly confined liquids. Here, the term strong confinement refers to situations where the dimension of the confinement (e.g., the distance between the confining walls) is as small as a few particle diameters. When dealing with molecular systems, this would correspond to nano-confinement, whereas in the case of colloidal suspensions, distances of a few microns already represent strong confinement. It is well-known that confinement has strong influence on the dynamics of glass forming materials and thereby on the glass transition itself. Albeit dependent on the specific wall-fluid interactions, this effect, however, was long thought to be monotonic with regard to a variation of the linear dimensions of the confinement. In other words, if the effect of a given substrate was to slow down the system dynamics and thus increase the glass transition temperature, the effect was observed to grow with increasing confinement (decreasing wall-to-wall separation). The same trend was also reported for substrates with an accelerating effect on the system dynamics. In this case, the stronger the confinement is, the larger is the resulting enhancement of the structural relaxation and the corresponding reduction of the glass transition temperature.

The violation of this trend in the case of strong confinement could be shown in a joint theory-simulation research effort in collaboration with our partners from the Universität Innsbruck (Thomas Franosch) and the Eberhard Karls Universität Tübingen (Martin Oettel). The main idea leading to this interesting finding is that introducing competing mechanisms may lead to glass transition phase diagrams exhibiting non-monotonic behaviour. Such a situation arises in the case of a liquid sandwiched between two planar hard walls. The confinement introduced by the walls sets a strong constraint for particle spacing in the direction perpendicular to the wall surface and thus competes with the commensurability of the liquid. It turns out that the variation of the wall-to-wall spacing creates fully commensurate to non-commensurate states in an oscillatory manner, whereby commensurate phases correspond to the integer multiples of the particle diameter. A consequence of this oscillatory variations of the packing structure with wall-to-wall separation is a corresponding non-monotonic variation of the system density and dynamics at the same constant chemical potential (or, equivalently, external pressure).

Fig. 5.16 provides an illustration of this effect for the case of wedge geometry. The use of wedge type geometry has the advantage that its realisation in experiments is rather straightforward. Moreover, the distance between the upper and lower walls changes with the distance from the edge point so that a range of wall-to-wall separations can be investigated simultaneously. This provides the attractive possibility of testing theoretical predictions on the non-monotonic confinement effects in a single experiment. As shown in *Fig. 5.16*, packing fraction shows a non-monotonic dependence on the wall-to-wall separation (realised by a variation of the distance from the edge point). The remarkable agreement between molecular dynamics simulation (MD) and density functional calculations using the fundamental measure theory (FMT) underlines the physical soundness of the obtained results. It is also seen from these studies that the non-monotonic effect becomes more enhanced at higher average packing fractions, which is controlled by the external pressure. Based on this observation, coexistence between glass and liquid regions may be achieved at sufficiently high pressures. This opens the way for various applications,

e.g., those making use of a mobility contrast between the glass and liquid domains and its controlled variation by the external pressure.

A comparison of the non-monotonic effect for the two cases of a polydisperse and monodisperse system reveals that density varies much more strongly in the monodisperse case than in the case of a polydisperse system (compare, e.g., the case of packing fraction φ=0.42 in the left and right panels). This observation supports the interpretation that the non-monotonic effect of confinement basically results from a violation of commensurability. Confinement has the strongest effect on commensurability if the system is monodisperse. In the case of a polydisperse system, smaller particles may play the role of interstitials and thus locally improve the degree of commensurability.

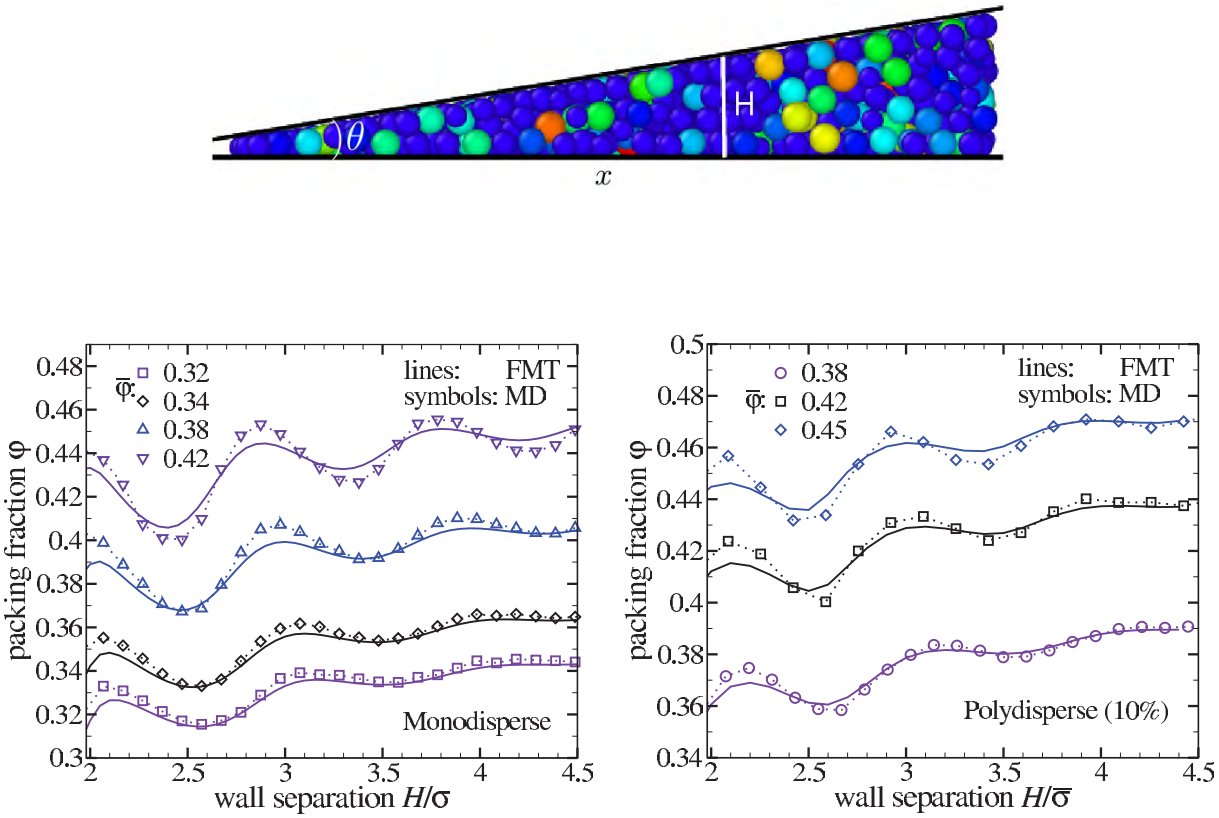


Fig. 5.16: Top: A snapshot of a typical wedge geometry studied via molecular dynamics simulations (MD) and fundamental measure theory (FMT). The system is a polydisperse hard sphere liquid. Particle sizes are drawn from a Gaussian distribution with 10% relative standard deviation. The height H varies with distance from the edge as H=x tan(θ). Bottom: Variation of the local packing fraction with the thickness of the channel for a monodisperse (left) and a polydisperse (right) hard sphere fluid for a number of average packing fractions as indicated. The plots compare results obtained from molecular dynamics simulations (MD) with a density functional approach using fundamental measure theory (FMT). The local packing fraction is determined within slabs of thickness dx = 1 particle diameter. The average packing fraction is controlled by the external pressure.

A further example of research topics explored recently in the complex fluids group is the nature of diffusion induced by an external perturbation such as an external shear. Imposed shear is well-known to give rise – in addition to the flow – to a stochastic motion. Due to relatively fast thermal motion in liquids, this shear-induced stochastic motion does not influence the system properties. For example, the diffusion coefficient or viscosity in the normal liquid state is hardly affected by shear so that these transport properties can safely be assumed to be independent of the external perturbation. This is exactly the well-known case of Newtonian liquids which show a linear response behaviour, where the response of the system (e.g., shear stress) is linearly proportional to the external perturbation (e.g., imposed shear rate) with a constant of proportionality (viscosity in this example) that is independent of the perturbation.

This situation changes qualitatively if thermal fluctuations are not strong enough to induce significant diffusion over the experimental time window. An amorphous solid (glass) is a good example of such an 'athermal' system. Other examples are systems made of large particles, so that thermal motion of particles can be neglected. Granular matter and suspensions of large vesicles and capsules belong to this category. In these systems, particles do not move in the so called quiescent state, i.e., in the absence of external perturbation. When exposed to an external shear, collisions between particles take place, thereby giving rise to a stochastic motion. Since the collision rate increases with density/packing fraction, this also reflects itself in a dependence of the stochastic motion on density. The effect of density becomes quite remarkable close to the jamming transition, where particles are in close contact and many body encounters become increasingly important.

As a typical example of athermal systems with biological relevance, we have investigated the above introduced concept of externally induced stochastic motion in dense suspensions of red blood cells. For this purpose, we have designed a simulation method to study the dynamics of dense suspensions of deformable particles in an ambient fluid in recent years. A deformable particle in the model is made of a closed membrane containing a liquid inside. While the forces acting on the membrane are obtained from a FEM calculation, the dynamics of the ambient fluid are updated by the Lattice Boltzmann method. The membrane-fluid coupling is realised via the immersed boundary method. Using this simulation methodology, we have thoroughly investigated the shear-induced stochastic motion in dense suspensions of red blood cells. Using the idea that the energy input by external shear is dissipated into heat within the ambient fluid in the small gaps between the red blood cells, a model could also be developed which relates diffusion to the viscosity of the system. One of the predictions of this model is that the diffusion coefficient is proportional to the square root of the suspension viscosity. This result is in good agreement with simulations.

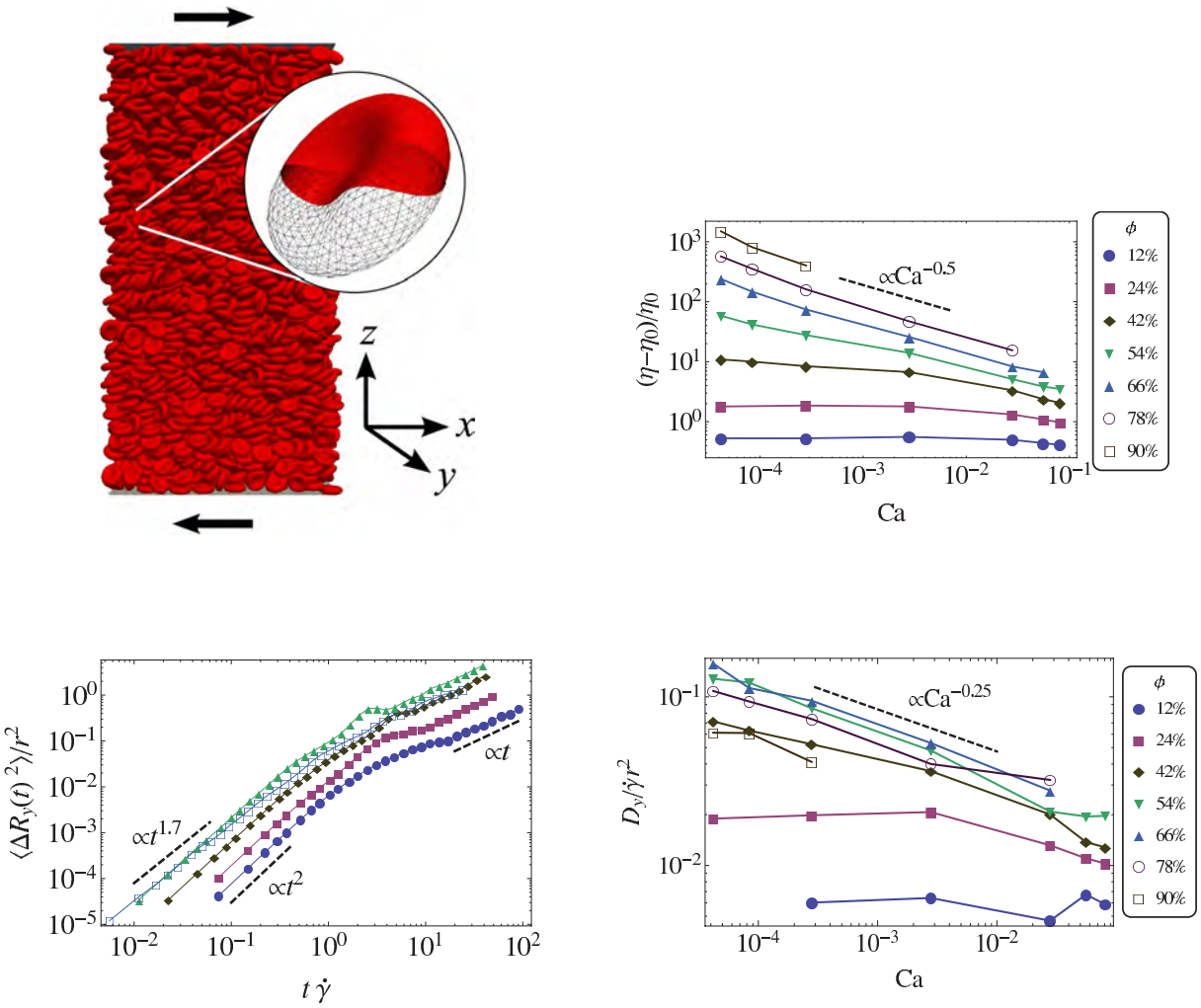


Fig. 5.17: Top: A snapshot of the simulation cell under constant shear (left) and the obtained results on the suspension viscosity, η, for various packing fractions as indicated (right). Ca is the capillary number, a dimensionless measure of the imposed shear. η_0 is the viscosity of the ambient fluid. Bottom: Computer simulation results on mean-squared displacement (left) and the diffusion coefficient (right) for different packing fractions as indicated in the legend of the right panel. MSD is scaled by the square of the average particle diameter, r. The diffusion coefficient D is scaled by the inverse shear rate. D is obtained from fits to the late time behaviour of the data in the left panel (the part linear in t). A close survey of the data shown here reveals that the diffusion coefficient is proportional to the square root of viscosity, $D \sim \eta^{0.5}$, at all packing fractions investigated.

STKS

5.4 Solid-Solid Interface Kinetics

Group leader:
Dr.-Ing. Reza Darvishi Kamachali

Group members:
Christian Schwarze

Introduction

The recently formed group focuses on the microstructural evolution within solid state materials. Our recent researches are concerned with grain growth, particle drag/pinning, recrystallization, and phase transformation in polycrystalline materials. The phase-field approach, which offers a wide range of possibilities for studying interface phenomena, is employed for studying sample volumes of materials with predefined thermodynamics and boundary conditions. Combining this method with mean-field theories provides a powerful tool to search for the grounds of physical events in the system of interest. This will allow for an understanding of macro processes in materials and for predicting the consequences of those processes in the functional properties of the product.

Research highlights

Revisiting mean-field theory of grain growth

Grain growth in the idealised polycrystalline body has been a topic of high theoretical and experimental interest for a long time. A fundamental problem in this field is the evolution of grain size in a polycrystalline and the existence (or non-existence) of self-similar solution(s) for the grain size distribution with respect to a characteristic length.

Motivated by our recent phase-field simulation results, the mean field theory of three-dimensional normal grain growth is revisited. In contrast to the theory of ripening, where the steady-state is enforced by thermodynamic conditions, we have found that the multiple self-similar regimes of grain growth exist and are determined solely by the geometrical relation between neighbouring grains. The size distribution function follows a single parametric form of

$$P(\rho) = 3e^{\frac{3}{2}c_\gamma} \frac{\rho}{(\rho^2-\gamma\rho+\gamma)^{\frac{5}{2}}} \exp\left(-\frac{3\sqrt{\gamma}}{\sqrt{4-\gamma}}\arctan\frac{2\rho-\gamma}{\sqrt{\gamma(4-\gamma)}}\right),$$

if $\rho=\frac{R}{R_{cr}}$ and c_γ are a constant. *Fig. 5.18* compares the above equation with our phase-field simulation results.

An index $\frac{\langle R\rangle^2}{\langle R^2\rangle}=\langle\rho\rangle$ is proposed and shown to be in a direct correlation with mean field parameter γ and the geometry of grains. Though it is difficult to characterise the geometrical features of grains, this index is easy to measure from numerical or experimental procedures. *Fig. 5.19* presents the evolution of this index along the simulations. One can see that a self-similar regime is approached for γ≈3.

Stretchability and texture evolution in AZ31 magnesium sheets

Due to their light weight, high specific stiffness, and strength, magnesium alloys are promising materials to be used across a wide range of applications from aerospace to automotive industry. Their capability, however, is challenged by limited plastic formability, which is directly related to the HCP structure of magnesium.

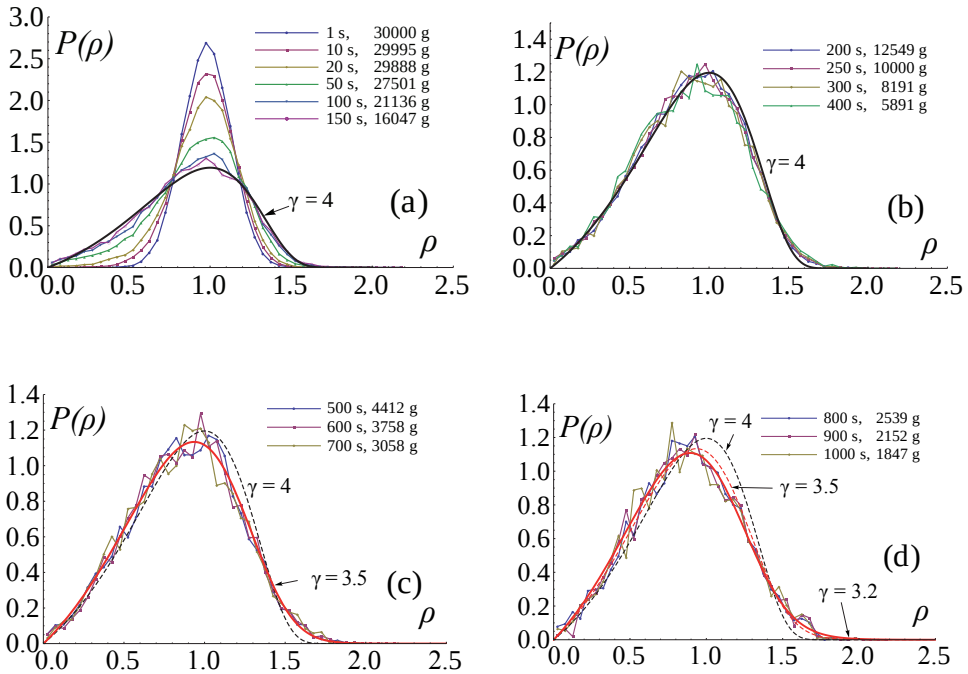


Fig. 5.18: Phase-field simulation results vs. the mean-field equation for grain size distribution.

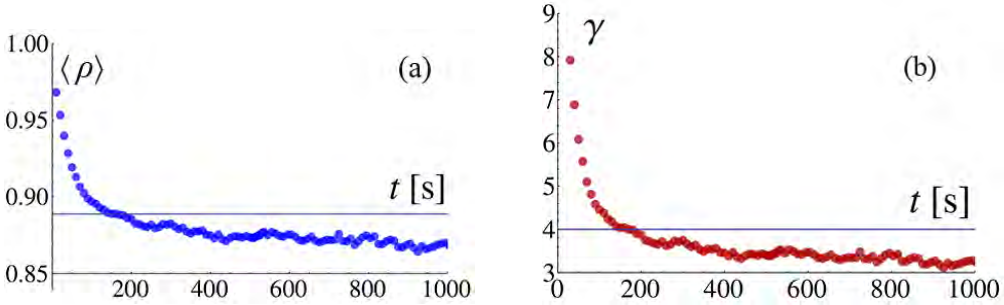


Fig. 5.19: Evolution of the index $\frac{\langle R\rangle^2}{\langle R^2\rangle}$ (a) and the mean-field parameter γ (b) along the simulation.

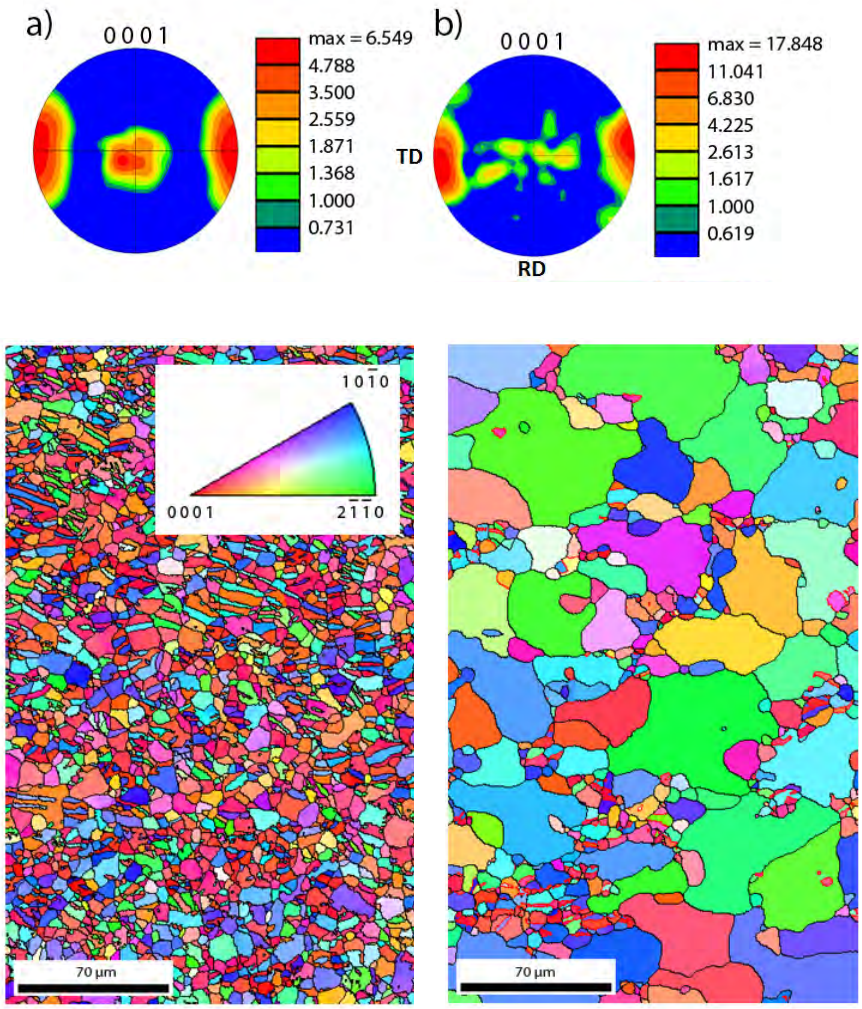


Fig. 5.20: EBSD analysis before and after annealing. The non-basal texture developed largely as a result of recovery and grain growth.

In collaboration with our experimental partner Dr. Se Jong Kim from the Korean Institute of Materials Science (KIMS) in South Korea, we have studied the formability in commercial AZ31 magnesium thin sheet. Combing in-plane plastic deformation of about 5% with a subsequent annealing at 573 K, a large improvement in the stretchability of the sheet has been observed. *Fig. 5.20* shows the experimental results.

The EBSD analysis combined with phase-field simulations shows that the static recrystallization during annealing of pre-compressed specimen is driven mainly by a local difference between stored mechanical energy in the neighbouring grains. *Fig. 5.21* shows the simulation results. At the beginning of annealing, untwinned grains with basal texture, which are thermodynamically unstable, are quickly consumed by twinned (sub)grains at the lowest stress state. In contrast to the normal grain growth simulation, which does not change the mixture's ratio, the stress-driven growth mostly favours the {2 $\bar{1}$ $\bar{1}$ 0} texture (green). These grains continue to expand by curvature-driven normal grain growth in the later stages of the annealing. At the presence of low-mobility twin boundaries, the twinned grains evolve slowly and other non-basal textures (grey), which are still in a relatively lower stress state, grow at the expense of the initial basal texture. The results of our study are under review for publication.

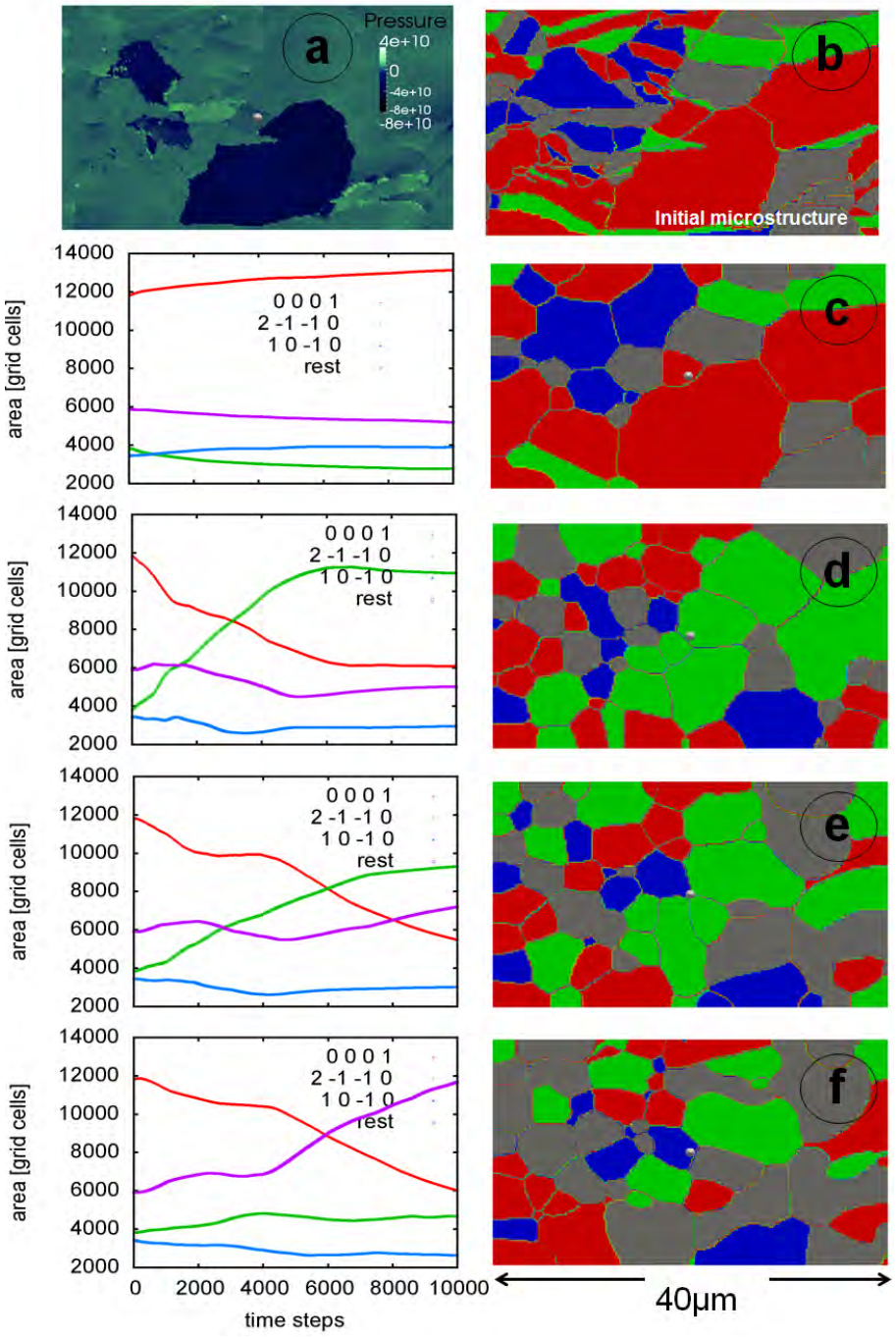


Fig. 5.21: Initial pre-compressed sample (stress state) (a, b), normal grain growth (c), stress-driven growth (d) and stress-driven growth including limited mobility of twin boundaries (e, f).

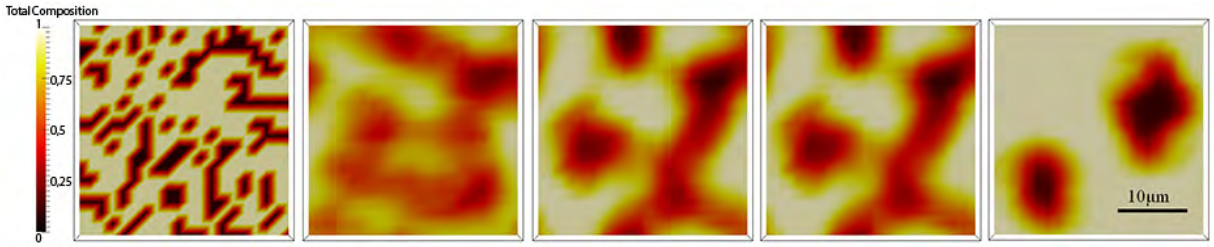


Fig. 5.22: Spinodal decomposition of copper-rich precipitates in Al matrix.

Precipitation in Al alloys

In the context of the recent SPP1713 program, we began to study precipitation in the Al-Cu-Li system. The early stages of growth, which are believed to be based on spinodal decomposition, are simulated by using a recent phase-field model of Steinbach et al. The results are shown in *Fig. 5.22*. In the current stage, growth of the δ' (Al_3Li) phase is considered. Our aim in to understand the mutual interaction between chemical and mechanical energy profiles around the precipitate. In the near future, the basic interaction between the precipitates and the role of external load will be investigated.

Particle pinning in polycrystalline materials

Particle pinning is considered one of the main effects of secondary-phase particles on the kinetic of grain boundaries. In our recent study we focus on the dynamics of particle/interface interaction and investigate the role of particle shape. We found that needle shape particles, such as carbon nanotubes (CNTs), may favour drag/pinning in particular situations. *Fig. 5.23* shows the diagram for effectiveness of particle drag.

Large scale simulations with 4 vol. % CNT show that shorter CNTs have a stronger drag effect and increase the growth exponent (i.e., retarded coarsening). *Fig. 5.24* and *Fig. 5.25* show the simulation box and the kinetics of growth, respectively. The results of this study are to be published in the near future.

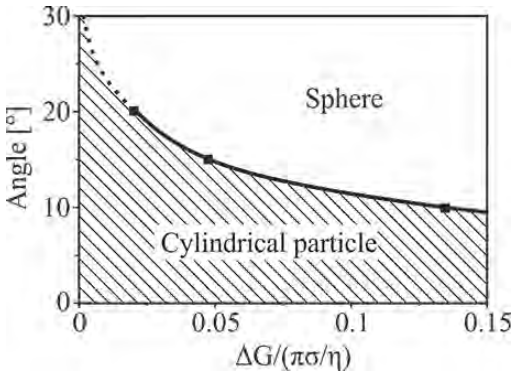


Fig. 5.23: The relative angle with respect to the interface and the driving force of the interface determine the effectiveness of cylindrical particles compared to spherical particles.

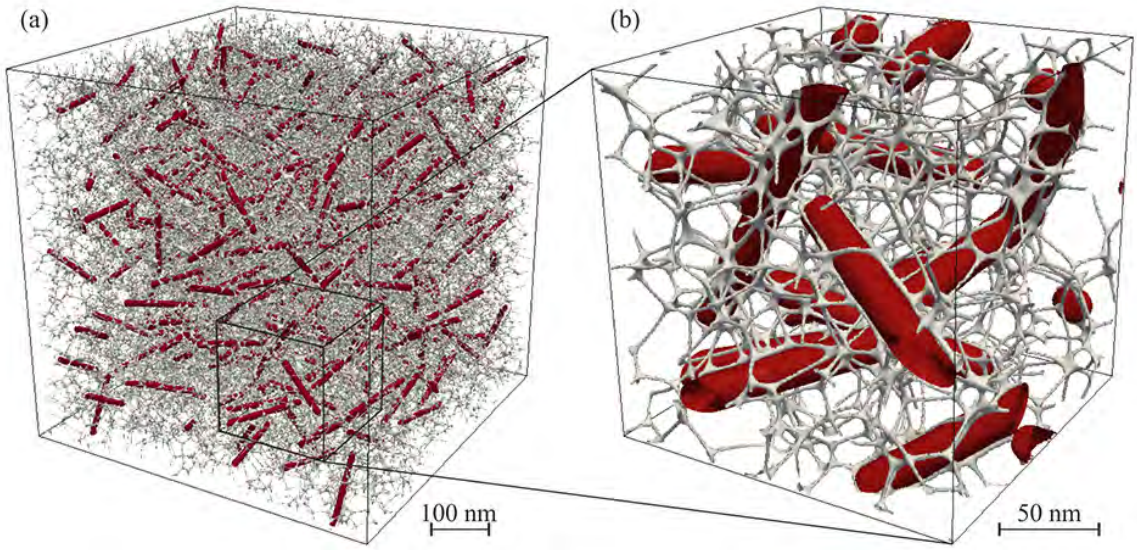


Fig. 5.24: Simulation box for long CNTs. Long CNTs have extended interaction with triple junctions.

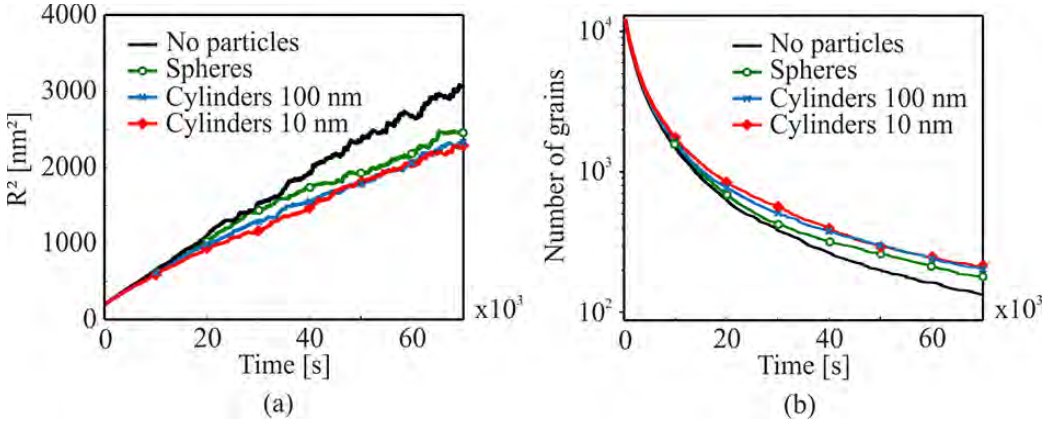


Fig.5.25: Kinetics of growth and number of particles for large scale simulations.

Department Micromechanical and Macroscopic Modelling MMM

6. Department Micromechanical and Macroscopic Modelling

Prof. Dr. Alexander Hartmaier

Research

Understanding and describing the relationships between the microstructure of materials and their macroscopic mechanical properties is the main research objective of the research activities within the Department Micromechanical and Macroscopic Modelling (MMM). Our research is motivated by the need to tailor material properties that meet the demanding requirements of their designated application in modern engineering structures. The production of such materials on an industrial scale requires robust and efficient thermomechanical processes. A thorough physical understanding of the critical mechanisms occurring during thermomechanical processing as well as during the application of materials demands for a scalebridging approach as it is established within ICAMS. Only scalebridging models will have the predictive power needed for a robust material and process design to support the optimization of existing materials and, moreover, for the time and cost efficient development of novel materials with unprecedented properties.

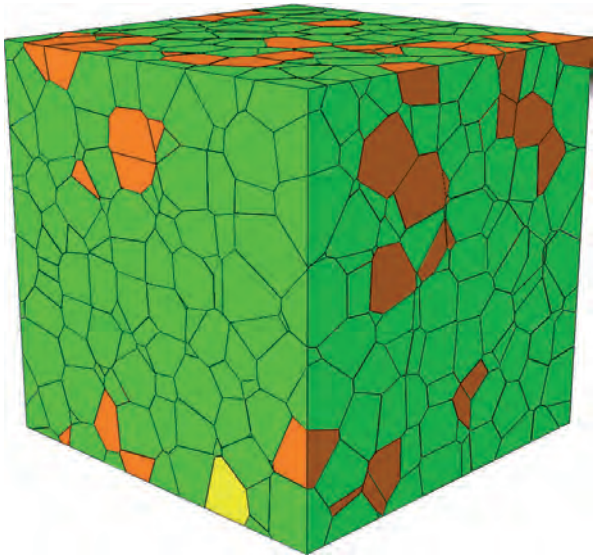


Fig. 6.1: Representative Volume Element (RVE) of a polycrystalline material containing several phases. In this model of a dual phase steel, green grains represent ferrite, orange grains represent retained austenite and the yellow grain represents martensite.

Employing the methods of scalebridging material modelling allows us to deduce microstructure-property-relationships and thus to predict the mechanical properties of materials (strength, hardness, deformability, fracture toughness) as a function of their microstructure, i.e., as a consequence of their thermomechanical processing. Deriving the macroscopic mechanical behaviour of a material directly from its microstructure is possible by numerically characterising the mechanical properties of so-called representative volume elements (RVE), see *Fig. 6.1*. This approach examines the microstructure of a material within a volume large enough to capture all phases occurring in a material with a given microstructure described by volume fractions and size distributions of all phases and also the orientation distribution of individual grains within the phases. At the same time, the volume has to be as small as possible to allow for an efficient numerical description;

hence the name representative volume element. In an RVE, all phases and even individual grains are modelled explicitly and hence are represented by several finite elements. This method has proven to be a powerful tool in deriving mechanical properties resulting from realistic microstructures.

However, predicting material behaviour in a quantitative sense requires the a priori knowledge of the microstructure and also of the properties of all phases, their interfaces and the grain boundaries. The development of methods for obtaining a proper characterisation of realistic microstructures and local material properties has been one vital focus of the research in our department. In both cases the scalebridging modelling provides critical input in terms of physically sound models of elementary processes during microstructure evolution and also in terms of predicting properties of single phases from first-principles. The latter task is achieved by a close collaboration of MMM and mainly the group Mechanical Properties of Interfaces with the Department Atomistic Modelling and Simulation (AMS). However, since even scalebridging approaches will not be able to determine all material properties needed as input parameters for the micromechanical modelling, we also collaborate closely with the experimental Advanced Study Groups Input Data and Validation (RUB) and Processing and Characterization (RWTH Aachen).

A further advantage of the RVE method is that microstructure evolution during deformation can also be taken into account explicitly. Thus, the restriction from which many mechanical models suffer, namely to study only static microstructures, can be overcome. In a joint research effort with the Department Scalebridging Thermodynamic and Kinetic Simulation (STKS), advanced crystal plasticity models that take into account dislocation density evolutions are combined with the phase-field code OpenPhase developed in the Department STKS.

The department MMM is organised into three research groups, namely "Mechanical Properties of Interfaces" (Rebecca Janisch), "Crystal Plasticity Modelling and Simulation" (Anxin Ma) and "Discrete Micromechanics and Fracture" (Martin Boeff). In the year 2014 Dr.-Ing. Benjamin Reinholz successfully completed his PhD thesis, his work is briefly summarised in the report of the group Discrete Micromechanics and Fracture below.

MMM

6.1 Mechanical Properties of Interfaces

Group leader:
Dr. Rebecca Janisch

Group members:
Dr. Sankari Sampath
Dr. Xueyong Pang
Dr. Arshad Tahir
Dr. Karthikeyan Chockalingam
Mansour Kanani

The research group "Mechanical Properties of Interfaces" investigates the parameters which determine interfacial strength and deformability in metals and alloys on the atomistic scale. These physical properties, together with parameters such as interface geometry and chemical composition, are related to the deformation mechanisms that occur at interfaces during deformation of microstructures.

Ab initio electronic structure calculations based on density functional theory are used to predict the energy, strength, and elastic modulus of interfaces and other defects in metals and alloys. These characteristic properties are used to derive trends and constitutive relationships, as well as benchmarking empirical potentials for large-scale molecular dynamics simulations. Such dynamic simulations are carried out to determine fundamental deformation mechanisms – interfacial sliding and/or migration, dislocation emission, twinning – at different interfaces and temperatures during tensile and shear load. These mechanisms are then related to fundamental physical properties.

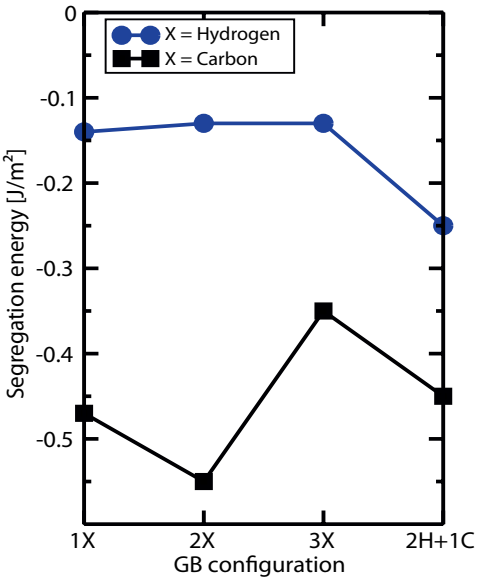


Fig. 6.2: Segregation energies of interstitial elements at the Σ5 symmetrical tilt grain boundary in iron.

In 2014 the projects of the work group focused on the effect of alloying elements and impurities (Si, C, H) on the deformability and strength of ferritic steel (S. Sampath, A. Tahir, and K. Chockalingam), and on the effect of temperature and interface structure on the deformation mechanisms in aluminium and titanium-aluminium alloys (X. Pang and M. Kanani).

An ab initio study of the effect of hydrogen on grain boundary cohesion in iron revealed that hydrogen enhanced decohesion (HEDE) is a potential source of hydrogen embrittlement in ferritic steel if it is understood as an effect of co-segregation of carbon and hydrogen at the interface. The calculated segregation energies are negative for both individual elements, C and H, at a Σ5 symmetrical tilt grain boundary in body centred cubic Fe, as shown in *Fig. 6.2*. This is especially true for carbon due to its extremely low solubility in the bulk crystal. Thus, the C segregated state can be considered the ground state of this grain boundary, provided there is a sufficient amount of C in

the material. However, the situation changes when H is available as well. When taking grain boundary segregation with either 3 H or 3 C atoms as reference (corresponding to coverage of 0.75 monolayers), the segregation energy can be lowered further by partially replacing one element by the other. The example in *Fig. 6.2* shows the segregation energy for a combination of 2 hydrogen atoms with 1 carbon atom. This co-segregated state is thus always preferred over those states with only one type of elements, including the one with 3 C atoms.

The effect of the co-segregation on the fracture strength of the Σ5 grain boundary is visualized in *Fig. 6.3*. Referred to the interfacial strength in pure Fe, hydrogen has a negligible effect. This can be understood by a look at the electronic structure (not shown) at the grain boundary, illustrating that H, when placed in the open structural units of the interface, hardly interacts with Fe at all. This is totally different for C, which forms directional bonds with the matrix and strongly increases the grain boundary cohesion. The strength is reduced again if C is partially replaced by H, a process that is favourable from an energy point of view, as explained above. In this sense, H can cause enhanced decohesion at this interface in ferritic steel by supplanting the alloying element C.

The dynamical shear behaviour of grain boundaries in aluminium and aluminium alloys has been investigated by means of molecular dynamics simulations using embedded-atom method type potentials. Shearing different bicrystals of face-centred cubic Al as well as of γ-TiAl

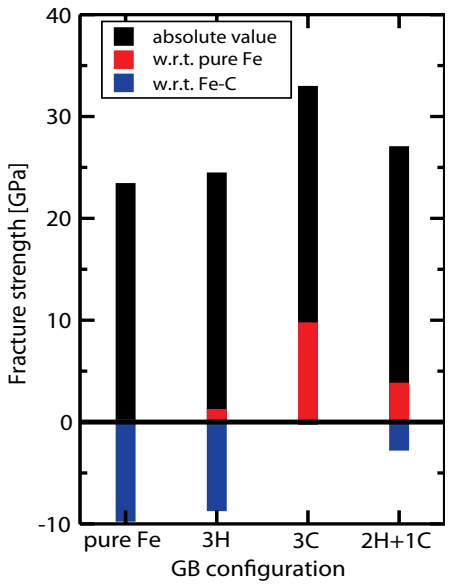


Fig. 6.3: Fracture strength of the Σ5 symmetrical tilt grain boundary for different configurations of segregated interstitial elements H and C at the interface.

revealed several deformation mechanisms. While in Al there is a competition between mechanisms that result in rigid grain sliding and dislocation emission from the grain boundary into the bulk, no such thing is observed in TiAl. While this material also shows a variety of deformation mechanisms, they all leave the grain interior intact. This is attributed to the slight tetragonality of the structure, which reduces the number of slip systems for crystal dislocations compared to the perfect face-centred cubic one.

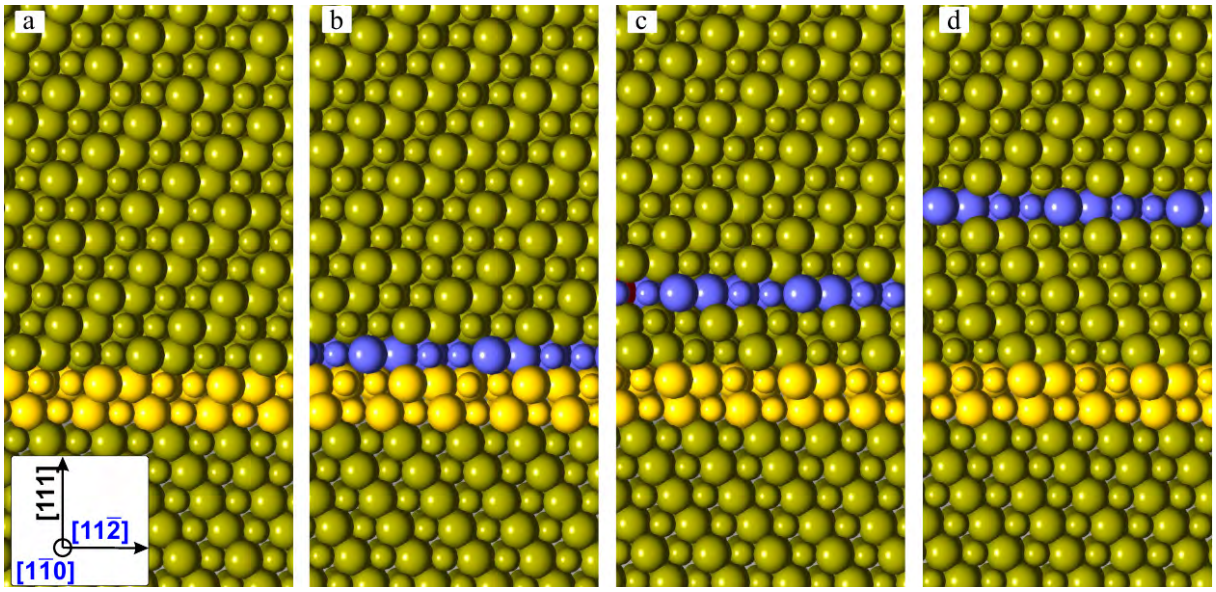


Fig. 6.4: Snapshots of a molecular dynamics simulation of shear at a (111) 60° rotational boundary in TiAl. Yellow atoms mark the interface, blue atoms the twin boundary which is nucleated and migrates into the upper grain.

Another remarkable difference between TiAl and Al is observable at the (111) 60° twist grain boundary. When sheared along the [11$\bar{2}$] direction, the bicrystal accommodates the shear strain by grain boundary migration in case of Al. In TiAl, however, a second planar defect is nucleated which then migrates instead of the interface. Some snapshots of this process are shown in *Fig. 6.4*. The underlying twinning mechanism is known to occur in single-crystal TiAl as well. The fact that it does not happen at the geometrically equivalent interface in Al can be traced back to differences in the generalized stacking fault energy (GSFE) surfaces of Al and TiAl. A detailed study of such GSFE surfaces additionally provided explanations for the other deformation mechanisms at grain boundaries. This enables us to create direct links between material properties and deformation behaviour and thus to evaluate the effect of alloying elements on dynamical processes even with ab initio calculations.

The effect of silicon on the carbon solubility and mechanical properties of a bainitic steel is investigated in the framework of a collaborative research project with industrial and academic partners. The goal is to understand the reason for the supersaturation of bainitic ferrite with C, which is being observed experimentally, as well as the influence of Si on the tensile and shear strength of the materials. In both sub-topics, C solubility and strength, unexpected effects due to the Si-C interactions are observed. By way of illustration, *Fig. 6.5* shows snapshots of the Σ3 twin boundary in body centered cubic Fe under tensile load. The structure is shown a) for pure iron, b) for the case that the Fe layer forming the boundary is replaced by silicon and c) with additional interstitial carbon atoms at the boundary. The local atomic structure for comparable tensile displacements differs significantly for the three compositions. Especially in the case of the ternary system, Fe-Si-C, the variation of the Fe-Si and C-Si bond angles leads to metastable states with comparable energies. The impact of such states on the mechanical properties will be subject of further investigations.

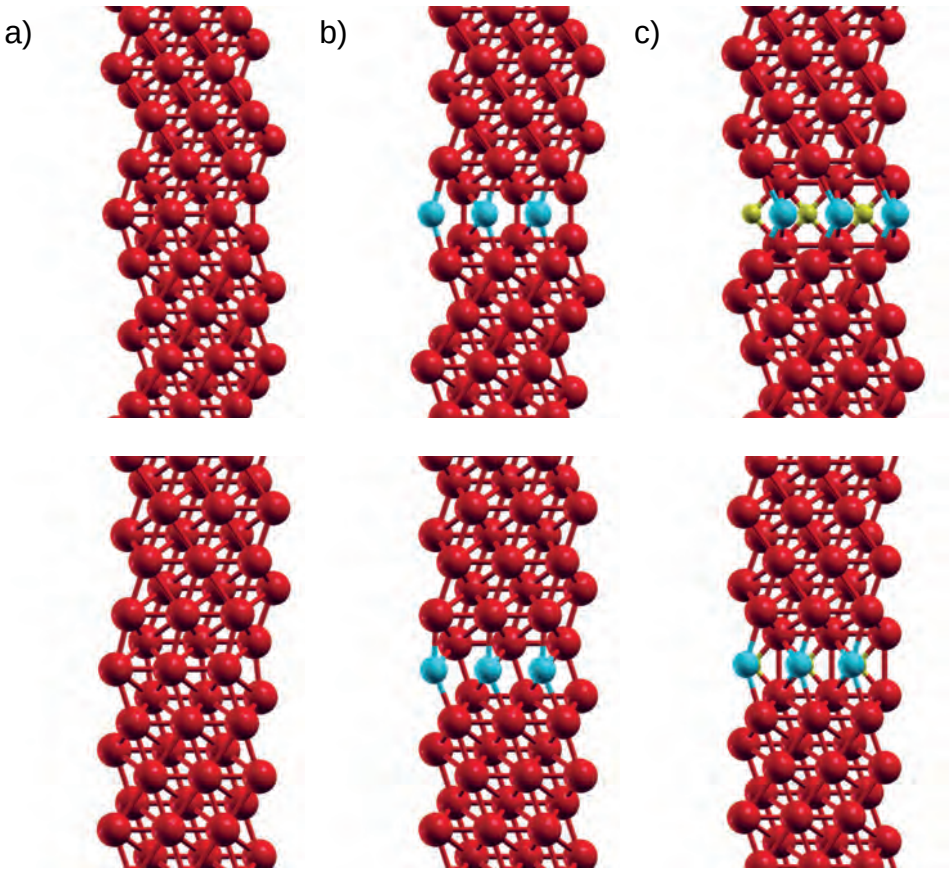


Fig. 6.5: The Σ3 twin boundary a) in bcc Fe, b) with the grain boundary atoms substituted by Si (turquoise), c) with additional interstitial carbon (yellow). The upper row shows the structures under 1% tensile strain along the vertical axis, the lower row shows the grain boundaries under 3% tensile strain. In a) and b), the tensile strain is partially accommodated by a shear displacement of the grains, while in c) this only happens for the Si sublattice.

MMM

6.2 Crystal Plasticity Modelling and Simulation

Group leader:
Dr.-Ing. Anxin Ma

Group members:
Philipp Engels
Siwen Gao
Satyapriya Gupta
Rehman Hameed

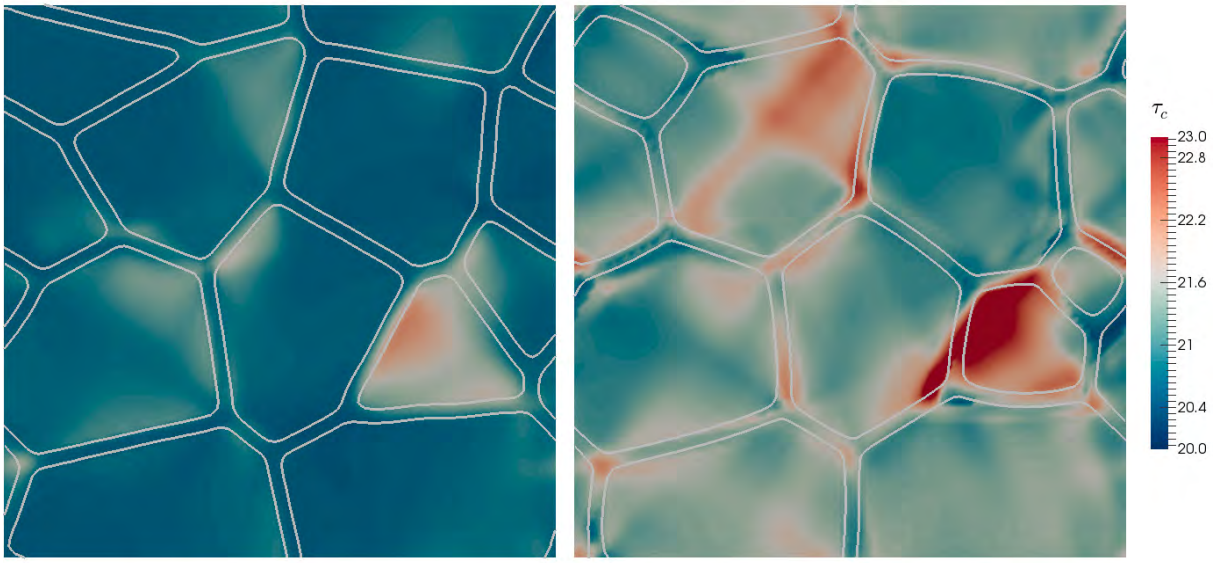


Fig. 6.6: Evolution of the crystal plasticity hardening parameter during grain-growth of a polycrystal under 10% eigenstrain.

The major goal of this research group is building and applying a micromechanics modelling platform for multiphase polycrystalline engineering materials, e.g., TRIP steels and nickel-based superalloys. This platform supports plastic flow, work hardening, and damage evolution laws based on microstructural mechanisms within a continuum mechanical framework. At the same time, this group focuses on the development of efficient numerical approaches for mechanical and coupled processes including elasto-plastic deformation coupled to atom and vacancy diffusion and phase transformations.

Dislocation density-based crystal plasticity model for phase-field simulation

During the thermal and mechanical treatment of alloys, martensitic phase transformations will cause internal stresses due to the volumetric strain and shape change of the crystal lattice. However, such increasing stresses are limited by the onset of plasticity, which is caused by the motion of dislocations in the corresponding phase. From an energetic point of view, this plasticity-induced limitation or reduction of the elastic free energy is expected to shift the ratio towards further energy contributions like interface and chemical energy and consequently varies the microstructure. In the

past year the large deformation framework of OpenPhase was finalised. The major addition was the full consideration of crystal lattice rotations during the on-going deformation process, which required the development of an interface model for orientation relationships in close collaboration with the OpenPhase developer team of the STKS department. Based on this model, rolling of elasto-plastic polycrystals was simulated in order to record texture development. With the established mechanical framework, the project's focus was consequently shifted towards processes including phase transformations. Therefore, the interaction between a moving interface and the field of hardening (or dislocations) had to be considered. Since the interaction is expected to rely severely on the respective type of grain or phase boundaries, extremal cases were implemented first, namely the full inheritance of dislocations and the full absorption of dislocations by the interface. The established implementation is highly optimized in order to deal with the severe demand of memory that will arise using the complex hardening models of typical crystal-plasticity models. *Fig. 6.6* shows an example of such a coupled simulation conducted by Philipp Engels. A randomly orientated polycrystal is exposed to anisotropic eigenstrain. During the following grain-growth, the material is exposed to significant yielding and hardening processes. All mentioned developments were presented at the European Mechanics of Materials conference in Gothenburg, Sweden, in August 2014.

Influence of microstructure on creep resistance of superalloy single crystals

In the last year Siwen Gao implemented several typical microstructures of single crystal superalloys, which are often observed in experiments and which recently have been successfully reproduced by phase-field simulations into her three-dimensional discrete dislocation dynamics (3D-DDD) simulations to study the influence of microstructure on material creep resistance. The misfit stresses due to the matrix/precipitate lattice mismatch in the complex microstructure were efficiently calculated by the Fast Fourier Transformation method (FFT). *Fig. 6.7* shows the simulation results for mainly athermal dislocation slip in the matrix channels. From comparisons of macroscopic mechanical responses and dislocation evolutions for different microstructures under constant uni-axial tensile load along different crystallographic directions, it was found that for the same precipitate volume fraction, the optimal deformation resistance occurs in the microstructure possessing narrow and homogeneous matrix channels.

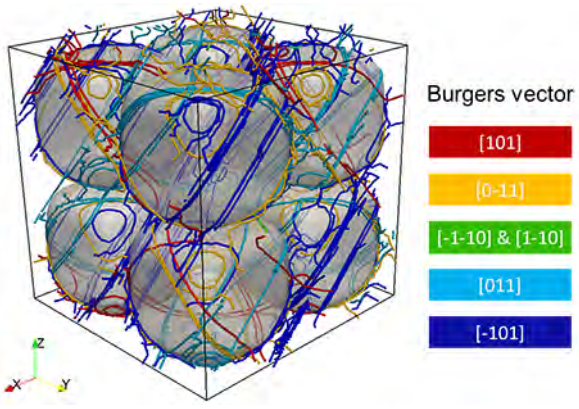


Fig. 6.7: Dislocation configuration in the microstructure with narrow and homogeneous matrix channels under constant tensile load along z direction.

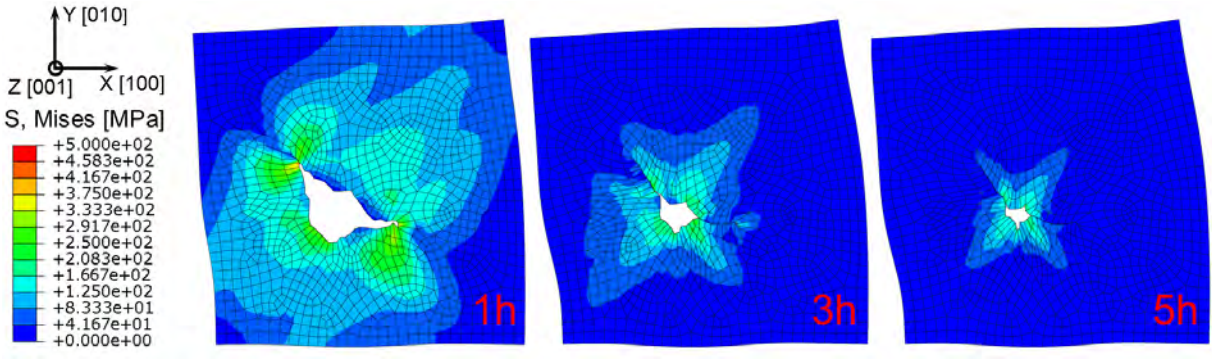


Fig. 6.8: Von Mises stresses and pore geometries predicted by CPFEM simulations for different holding times under 200 MPa isostatic pressure at 1200 °C.

Casting pore annihilation in HIP process

In order to find out the specific relationship between HIP parameters and casting pore annihilation and, furthermore, to optimize the HIP parameters, a quasi-two-dimensional crystal plasticity finite element model (CPFEM) was used by Siwen Gao to investigate the influence of different temperatures, isostatic pressures, and holding times on the porosity reduction in an as-cast Ni-based single crystal superalloy during hot isostatic pressing (HIP). The CPFEM creep model takes the typical matrix/precipitate microstructure, the various realistic pore morphologies, the internal stresses due to matrix/precipitate lattice mismatch, and the additional hardening produced by deformation heterogeneities into account. In this model, temperature influences the volume fraction of the precipitate, the atoms' self-diffusion coefficient as well as the initial and the saturated critical resolved shear stress. The experimental and simulation results achieved a good agreement on the porosity reduction kinematics, as seen in *Fig. 6.8*. It was found that increasing the HIP temperature or increasing the isostatic pressure could reduce porosity effectively. However, if the temperature is very high or the porosity level is very low, increasing isostatic pressure or prolonging the holding time does efficiently acelerate the pore annihilation. It was also found that initial pore geometry strongly influences the annihilation process. For example, under the same HIP conditions, larger pores always shrink faster than smaller pores with similar shape on the initial stage of the HIP process. Furthermore, it became obvious that the large precipitate particles adjacent to the pore retard the porosity annihilation.

Influence of grain boundary on martensitic phase transformation

Non-homogeneous plastic deformation across the grain boundaries can produce a significant amount of strain gradients, which can influence the kinematics of the phase transformation in the vicinity of the grain boundary. Crystal plasticity finite element model (CPFEM) simulations, which consider the additional hardening caused by strain gradients and the austenite-martensite phase transformation, have been carried out by Satyapriya Gupta to examine the influence of grain boundaries on the martensitic phase transformation and overall mechanical behaviour of metastable austenite steels. Contour plots in *Fig. 6.10* demonstrate the distribution of transformed volume fraction of martensite for local and non-local CPFEM simulations. It was found that the higher order non-local CPFEM simulation is able to capture the presence and influence of grain boundaries on the martensitic phase transformation. We observed the accelerated

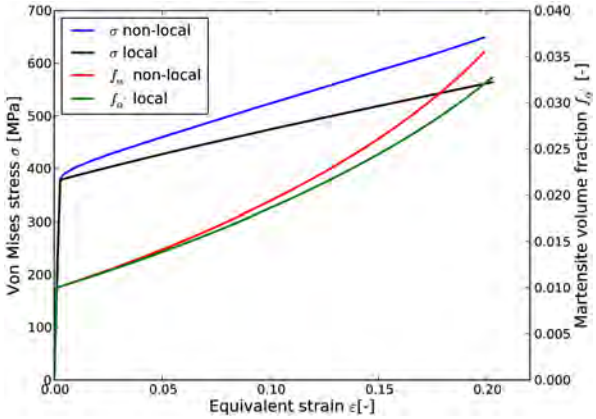


Fig. 6.9: Global stress and martensitic volume fraction obtained from local and non-local phase CPFEM simulations under uni-axial tensile deformation.

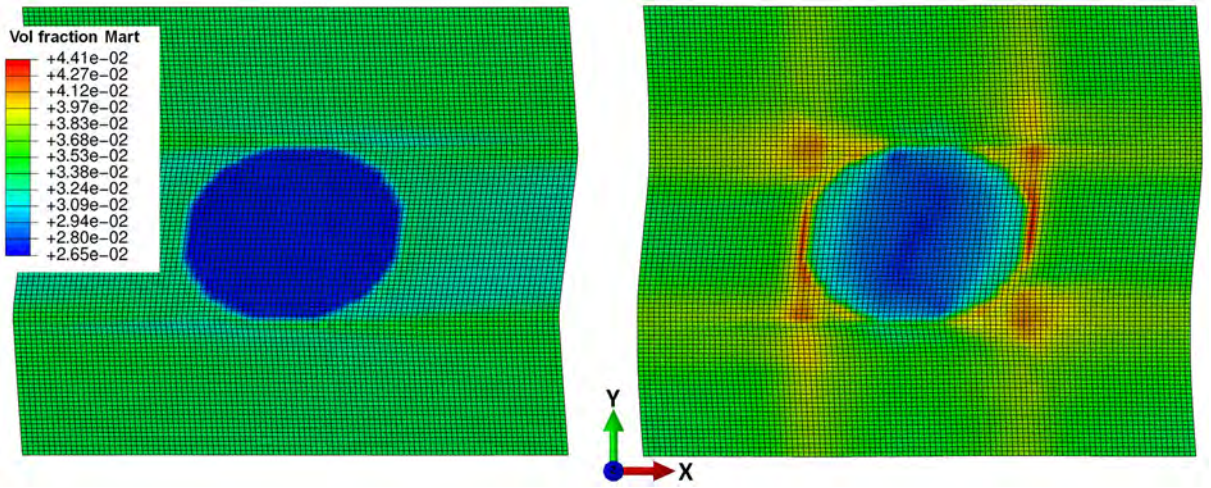


Fig. 6.10: Transformed volume fraction of martensite after 20% tensile strain in x direction. Left and right plots are the local and non-local CPFEM simulations, respectively.

kinematics of phase transformation in the vicinity of grain boundaries for non-local CPFEM simulation as compared to the local CPFEM simulation. This increase in the phase transformation speed must have a relation with the strain gradient hardening. The quantification of grain boundary influence on the averaged martensitic phase transformation and global stress state is presented in *Fig. 6.9*. A substantial difference in the stress magnitudes of nearly 100MPa is obtained from local and non-local CPFEM simulations, which is primarily caused by the enhanced hardening provided by plastic strain gradients and martensitic lamellar.

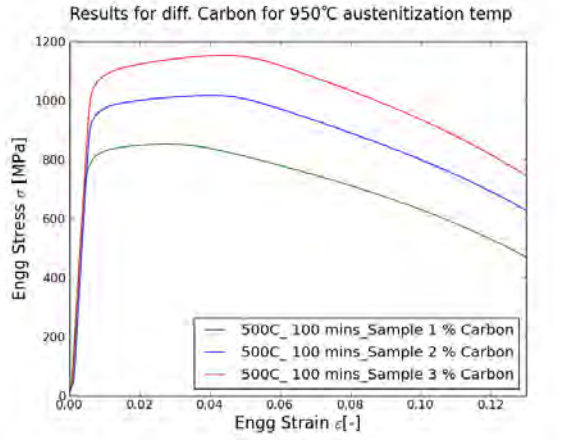


Fig. 6.11: Flow curves of tensile test for different carbon concentrations.

Micromechanical modelling of tempered martensite steels

In 2014 the mechanical properties of steel with a tempered martensitic microstructure have been be determined by Rehman Hameed by using CPFEM modelling and experimental techniques. A number of heat treatments and tensile experiments have been performed on tempered martensitic steel in order to study the temperature and carbon concentration dependence (austenitising and tempering temperatures) of prior austenite grain size and strength of the respective steel. *Fig. 6.11* shows the carbon concentration dependence of flow curves for an austenitisation temperature of 950 °C with annealing temperature of 500 °C for 100 minutes. *Fig. 6.12* shows the effect of tempering time on the stress strain curve for 0.2 % carbon concentration and an austenitisation temperature of 950 °C. It was found that increasing carbon concentration causes an increase in the yield strength. For higher tempering times, the material is showing more ductility but at the same time lower hardness, which is a well-known effect.

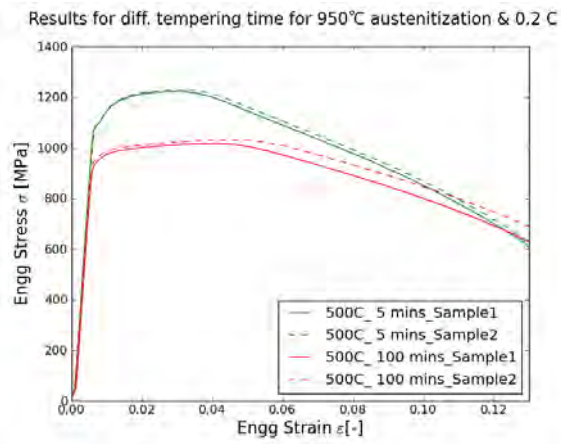


Fig. 6.12: Flow curves of tensile test for different tempering times.

MMM

6.3 Discrete Micromechanics and Fracture

Group leader:
Martin Boeff

Group members:
Philipp Schwittek
Dr. Arshad Tahir
Dr. Benjamin Reinholz
Matthias Kulosa
Jenni Zglinski
Xiaochen Song

Martin Boeff's group is working to gain an improved understanding of the influence of microstructure on deformation processes, damage, fracture, and fatigue. The focus is set on method development and application of existing methods to describe deformation processes on a physical basis. The research group mainly uses continuum mechanical methods.

During the year 2014 the research group had seven members. Jenni Zglinski is working within the Demonstrator project C2, where she investigates the micromechanical deformation properties of tempered martensite. Dr. Arshad Tahir finished his PhD in 2014 and joined the research group to take up the project of Dr. Dhiraj Mahajan, dealing with hydrogen embrittlement under cyclic loading conditions. Dr. Benjamin Reinholz finished his PhD in 2014 by revealing the influence of the microstructure of magnetic shape-memory alloys on the global deformation properties funded by the DFG. Matthias Kulosa investigates the deformation behaviour of porous ceramic material and its brittle failure in collaboration with a research project at the DLR in Köln. Philipp Schwittek investigates the influence of hydrogen on the failure mechanisms of martensitic steels using continuum mechanical methods. Xiaochen Song investigates the fatigue failure of martensitic steels and joined the research group in 2014.

Fracture and fatigue frequently lead to the failure of structural components, which might be followed by a loss of property or even human life. In metals like steel and aluminium, fracture is connected to the evolution of plasticity. One the one hand, vast amounts of plasticity lead to increased ductility and energy absorption shielding the propagating crack. On the other hand, mobile dislocations, which are the microstructural origin of plastic deformation, are lattice defects that cause irreversible deformation and damage nucleation under fatigue conditions. Therefore, crack initiation and propagation are governed by the competition of dislocation-induced crack shielding and irreversible damage caused by plastic deformation.

Jenni Zglinski proceeded with her work for the ICAMS Demonstrator project, in which she experimentally characterises the micromechanical deformation behaviour of tempered martensitic steel. Within the Demonstrator project, three types of tempered martensitic steel, differing in the carbon content (0.1, 0.2 and 0.3% C), are investigated. Her project combines experimental techniques to determine the deformation behaviour of martensitic steels and numerical techniques, using cohesive zone models to determine the crack initiation and propagation behaviour.

Within the experimental approach, special focus is set on identification of micromechanical deformation mechanisms on fracture initiation and propagation along phase- and grain-boundaries. Therefore, it is necessary to understand the influence of microstructural properties like grain-size, orientation or precipitations. In order to determine macroscopic deformation properties, Jenni Zglinksi performed tension tests on the Demonstrator project materials for varying austenitisation temperatures and different temperings. It was confirmed that higher carbon content leads to higher yield strength, higher ultimate strength and lower fracture strain.

Furthermore, it was shown that the tempering procedure as well as the austenitisation temperature influences these properties. Whereas the austenitisation temperature strongly influences the martensite morphology, e.g., prior austenite grain size, packets and laths, tempering has no influence on the morphology but strongly influences the macroscopic deformation behaviour. The reason for this is that the carbon distribution within the material migrates more intensively to phase- and grain-boundaries for longer tempering periods, which then effects dislocation slip. An EBSD image of the martensitic microstructure is given in *Fig. 6.13* below.

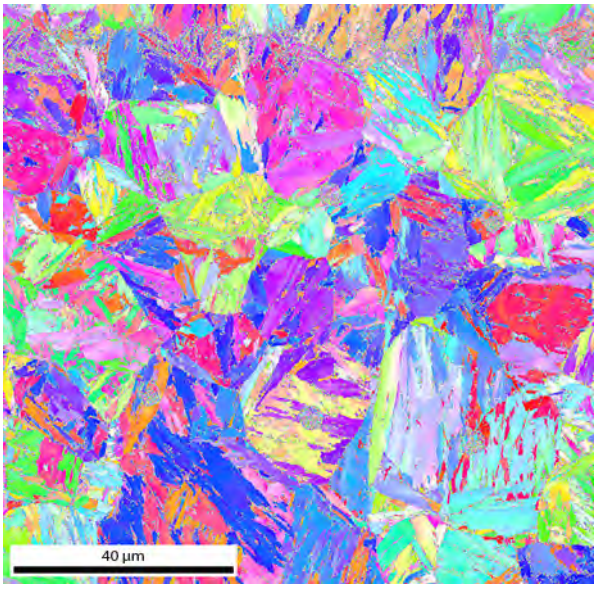


Fig. 6.13: EBSD image of tempered martensitic steel at an austenitisation temperature of 950 °C for 60 minutes.

Within this project, the microstructural deformation behaviour will be studied by nanoindentation. As a first approach to study the deformation behaviour of individual martensite-packets, single prior austenite grains will be indented in order to determine the influence of prior austenite grain orientation and variant distribution.

Jenni Zglinksi numerically investigated systematic crack initiation and propagation within a simple bi-crystalline material. The material parameters determining the traction separation behaviour of the material were initially taken from DFT calculations, but a broad parametric study followed to show the influence of each material parameter on the crack initiation period. In this study, the competing processes of plastic deformation at the crack tip, which is described by a J2-plasticity model, and the interface debonding at the grain boundary, which is described using a cohesive zone approach, is investigated.

Dr. Benjamin Reinholz finished his project on magnetic shape-memory alloys where he established relationships between the twin microstructure and the mechanical properties. Similar to ordinary shape-memory materials, magnetic shape-memory materials are so-called smart materials and are often used as actuators. Whereas the actuation frequency for ordinary shape-memory materials is limited as it depends on temperature changes, the actuation frequency of magnetic shape-memory alloys can be much higher. The magnetic field induced strain (MFIS), governing the magnetic shape memory effect, is induced by a rotating magnetic field and is based on the rearrange-

ment of crystallographic domains (twins) leading up to 20% transformation strain.

In order to study the deformation behaviour of magnetic shape-memory alloys, Benjamin Reinholz used discrete disclination dynamics, which are a further development of discrete dislocation dynamics specially tailored to describe twin boundary motion. Benjamin Reinholz showed the applicability of this method for describing the magnetic shape-memory effect and the determination of the stress-strain diagram during transformation. It was found that the MFIS and thus the stress-strain diagram are highly sensitive to the microstructure and to the motion of twin-boundaries. Using disclination dynamics, Benjamin Reinholz identified five characteristic regions within the stress-strain diagram of a magnetic shape-memory alloy: the elastic regime, the degressive region, the strain plateau, the progressive region and a second linear elastic region typically for shape-memory alloys (*Fig. 6.14*). The physical reasons behind these regions are identified using the disclination dynamics model which describes the twin motion and delivers a deeper understanding of fundamental deformation processes during twinning. The comparison with experimental results showed that the approach qualitatively describes the experimental findings.

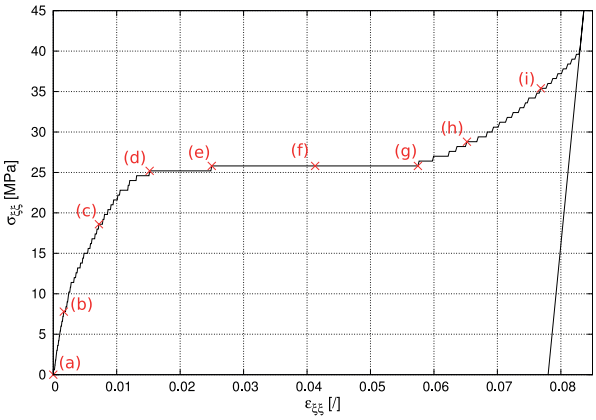


Fig. 6.14: The image shows a stress-strain diagram for a magnetic shape-memory alloy with its typical regions and a pronounced plateau (e-g).

Matthias Kulosa investigated the deformation behaviour and fracture properties of porous ceramics. Fibre-reinforced ceramics are well-known for their good thermal insulation properties as well as for their high mechanical strength and damage tolerance and are therefore applied in burners, gas turbines or other high temperature applications. Fibre-reinforced ceramics have a complex hierarchical structure, and consist of fibres and matrix material. Within his project, Matthias Kulosa is especially interested in the deformation behaviour of the porous matrix material consisting of sintered particles, as the implications of the matrix material on damage properties are not fully understood yet. A standard approach to correlate the mechanical properties of porous materials to microstructure is porosity. However, it is known that for a constant porosity there exists a broad range in which mechanical properties can differ. This evokes a preference for using a different quantity than porosity for the correlation.

From a combination of stochastic and mechanical modelling, Matthias Kulosa derived a new microstructural parameter for the characterisation of porous materials – namely the connectivity which is quantified by the average coordination number of particles sintered together. Within this approach, realistic representative volume elements of the porous matrix material are created with controlled microstructural features. It is now possible to consider porosity and connectivity independently. It is further shown that connectivity shows a substantial correlation with the homogenized Young's modulus of the material, while for a constant average coordination number the influence of the porosity is small.

As a second step, Matthias Kulosa implemented a brittle damage model and studied the damage initiation and evolution within a simplified porous matrix material. The deformation within the porous matrix material is very heterogeneous due to the complex morphology and the high stiffness contrast between material and air with high stress peaks at the sintering necks. Dominant load paths which carry the majority of the load are identified. It was found that zones sensitive to damage initiation are the sintering necks within highly loaded regions. Regions which are unstressed prior to damage initiation transfer parts of the load as the load paths change during damage evolution. As a next step, a more detailed study of the damage initiation and propagation on realistic porous RVEs will follow to provide detailed insight on the influence of porous microstructure on damage properties.

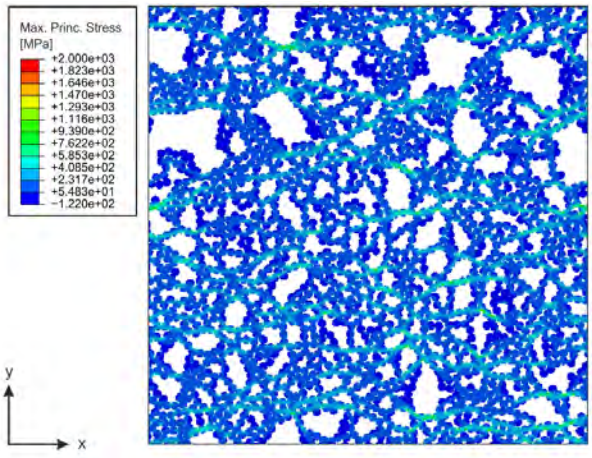


Fig. 6.15: The maximum principle stress is plotted within the RVE representing the porous microstructure where pronounced load paths can be observed.

Philipp Schwittek investigates hydrogen embrittlement in martensitic steels. During his project, he implemented a hydrogen diffusion model that is capable of describing stress-assisted hydrogen diffusion and trapping. The hydrogen interaction with local plasticity and cohesive failure along grain-boundaries is studied.

A NACE Method D test of martensitic steel is simulated as illustrative example for structural materials suffering from hydrogen embrittlement. With the help of the hydrogen diffusion model, a cohesive zone model, and under the assumption that hydrogen destabilizes the cohesive properties of the material, Philipp Schwittek is able to determine important crack growth features in sour environment, like the final stress intensity factor, K-dependent stage I and K-dependent stage II crack growth rates.

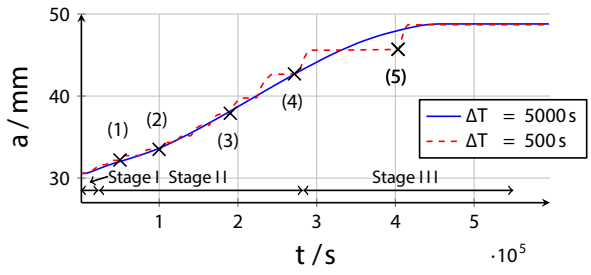


Fig. 6.16: The crack length is plotted over time for two different time steps, where the three stages of crack growth are marked.

An example of a simulated crack length over time diagram is given in *Fig. 6.16* for two different time increments used where the three stages of crack propagation are marked. The simulations further showed that the final crack length is mainly determined by the interaction of the stress intensity factor and the resulting stress-driven hydrogen accumulation, whereas the crack growth rate is mainly determined by hydrogen transport.

To gain a deeper understanding of microstructural features of martensitic materials and their role on hydrogen degradation, Philipp Schwittek implemented a model taking the prior austenite grain size and packet structure of martensite into account. Within this model, it is possible to evaluate the influence of prior austenite grain size, packet size and unfavourably oriented grains in form of weak and soft grains on the crack path and crack growth rate.

Martin Boeff explores the fatigue behaviour in steels based on the accumulated plastic slip. Within his project, he determined fatigue life times based on the accumulation of plastic strains during cyclic loading conditions describing the cyclic deformation behaviour of steels by crystal plasticity.

In order to study the damage evolution under deformation, he implemented a non-local damage model into a spectral solver. Due to the usage of the spectral method, it is possible to deal with complex geometries and to capture system sizes that are large enough to rectify the assumptions made when naming them representative volume elements. The well-known drawback of damage models to be pathologically mesh-dependent is resolved by using a non-local formulation in which the mesh dependency fully vanishes. Using this model, a dual phase model microstructure under monotonic loading conditions is investigated and regions susceptible to damage are identified. Additionally, three different regions in the resulting stress-strain diagram under uniaxial monotonic loading could be identified. While the first region is purely dominated by elastoplastic deformations, the second region is already influenced by damage initiation and evolution. The third region is the final failure region characterised by the coalescence of damage zones and formation of final damage bands spreading throughout the whole RVE.

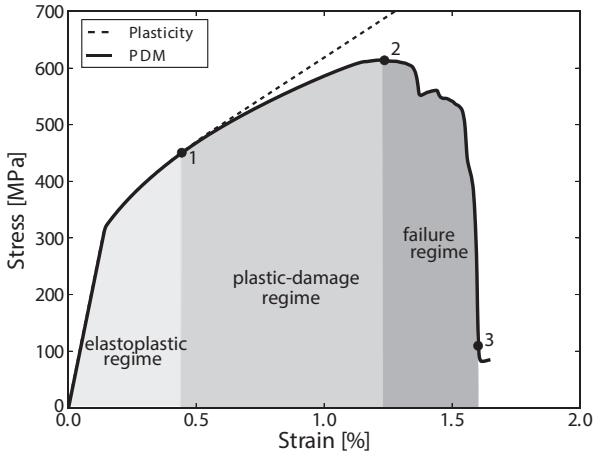


Fig. 6.17: A typical, simulated stress-strain diagram for the dual-phase steel shows three different regimes, namely the elas-to-plastic regime, the plastic-damage regime, and the final failure regime.

Furthermore, Martin Boeff develops an improved version of a martensitic RVE, taking martensite morphology, habit planes, martensite orientation relationships as well as prior austenite grain shape and orientation into account. With this model, it will be possible to study the complex influence of martensitic microstructural features on the deformation behaviour and to perform systematic parameter studies.

High Performance Computing in Materials Science

7. High Performance Computing in Materials Science

Group leader:
Dr. Godehard Sutmann

Group members:
Dr. Christoph Begau
Dr. Carlos Barjas-Teijeiro
Hariprasath Ganesan
Marvin Tegeler
Tao Wang

The research group led by Dr. Sutmann 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 has strong links to the other ICAMS departments and supports the development of simulation codes and efficient parallelization of programs developed at ICAMS. The current focus is on highly efficient implementations of bond-order potential methods, the combination of Monte Carlo and molecular dynamics (MD) in a parallel environment, parallel phase field simulations, large scale MD simulations on various systems, and the problem of load balancing for different methods.

The group was founded in 2012 and is financially supported by ThyssenKrupp Steel Europe. At present it is composed of six members. Dr. Christoph Begau was first to join the group after finishing his PhD at ICAMS in the field of dislocations in metals. Besides performing numerical experiments by MD simulations, he has developed a graphical analysis program for the structural analysis of solids that is frequently applied in the group and other departments. Dr. Carlos Barjas-Teijeiro, working as Postdoc joined the group in 2013. He is devoted to the parallelization of a bond-order potential code, originally developed at ICAMS and Oxford. The modular concept of the parallelization allows to integrate it as library into other atomistic simulation codes. Hariprasath Ganesan joined the group in October 2013 on a DFG grant. He is working on the diffusion of carbon in steel to understand the role of carbon on the dislocation mobility by means of a combined parallelization of molecular dynamics and Monte Carlo simulations. Marvin Tegeler also joined the HPC group in 2013 as a PhD student. He is working on the parallelization of the OpenPhase code, a program for phase field simulations, originally developed at ICAMS. Its efficient parallelization allows to extend computationally time demanding simulations, e.g., from 2D- to three dimensions. Tao Wang is close to finishing his PhD thesis in the group. During his work, he had a focus on large scale molecular dynamics simulations in the field of thermal transport and micro-structure analysis of metal and ceramic coatings.

The group has a strong link to the Supercomputing Centre Jülich, where additional large scale computing facilities are accessible. A benchmark simulation of the MD code IMD was conducted by the group in 2014 up to the whole capacity of JUQUEEN, an IBM BlueGene/Q architecture with more than 1.8 million compute threads.

Scientific interests of the group integrate activities from the three ICAMS departments AMS, STKS and MMM.

On the atomic scale, analytic bond-order potentials (BOPs) provide an efficient approach with linear complexity to accurately describe atomic interactions. They are derived from Density Functional Theory (DFT) and Tight Binding (TB) by applying the moments theorem to approximate the density of states in the system: every atom in the system samples a finite surrounding volume W_i and builds paths up to a given length m by hopping on the atoms included in W_i. The resulting large amount of path combi-

nations implies that BOPs are a very memory-demanding simulation, and thus it requires an efficient parallel implementation in order to obtain good scalability for large systems. The focus of recent developments has been put on two main areas: (1) the complexity analysis of the simulation code, which ensures the most efficient theoretical computation of BOPs is applied in the implemented code, and (2) the optimization of the parallel implementation, in order to make the results comparable to the sequential version for most test cases.

For fixed length of moment expansion m, the computation of paths presents a linear increase in simulation time with system size. However, longer paths are calculated, when improving the approximation level by increasing the length of the moment expansion, which implies a polynomial complexity with m. An accurate formulation of this progression has been obtained theoretically by relating the length of the paths to the volume explored during their computation. This complexity varies according with the number of moments, and has shown an asymptotic behaviour of $O(m^5)$ for an infinite path length m. For realistic approximation levels with m≈10, however, this progression is closer to $O(m^{4.5})$. After this analysis, the experiments with the BOPfox code have shown an almost perfect agreement with theoretical predictions.

The development of an optimal parallelization, based on a three-dimensional domain decomposition, focused on minimizing the number of operations required to compute all paths. As this scheme defines an overlap zone between every pair of neighbour domains, different coordination approaches have been tested, where the most efficient approach avoids all redundant computations and communicates the final interactions associated with every bond in the overlap zone between every pair of domains (*Fig. 7.1*).

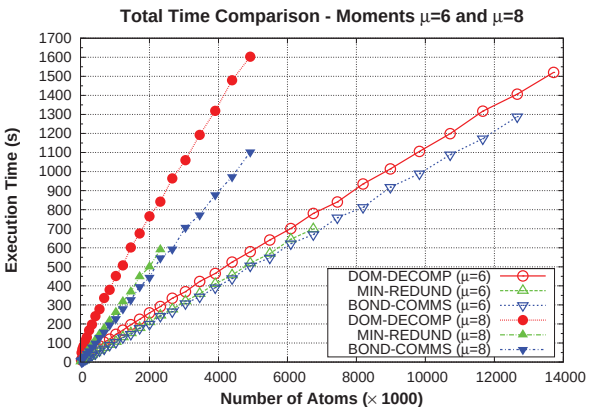


Fig. 7.1: Scaling behaviour of the implementation of bond-order potentials in BOPfox for different types of parallel algorithms. The most efficient algorithm, BOND-COMMS, avoids redundant calculations on neighboured processors.

The most efficient parallel version of the BOPfox code has been integrated in the main development trunk. Additionally, the code structure was redesigned to be integrated as external library into existing codes. An interface was written for the molecular dynamics code IMD, which originally implemented classical force fields and the embedded atom method (EAM). The inclusion of BOPfox therefore extends the functionality of IMD to calculate atomic potentials and forces on the basis of bond-order potentials.

Large scale particle simulations were conducted in the fields of dislocation dynamics, carbon diffusion and coatings.

The energies associated with dislocations and dislocation densities are frequently used as constitutive variables in crystal-plasticity modelling. Numerous but often contradictory models describing this functional have been proposed by various authors, derived from either theoretical or phenomenological considerations.

To clarify this discrepancy, the relationship between dislocations and the free energy was studied using Molecular Dynamics (MD) simulations. The advantage of these simulations is that they are only depending on the interatomic interaction and no assumptions need to be made to describe the deformation of crystalline solids. Thus, it serves as an ab-initio type approach where the dislocation density and free energy are directly measured.

A series of nano-indentation simulations has been performed in order to induce inhomogeneous densities of dislocations into pristinely defect free single crystals of aluminium. To quantify possible size effects, these simulations have been performed on approximately cubically shaped crystals with lateral sizes varying between 50nm and 150nm, consisting of about 7 to 200 million atoms. Especially in the latter case, the considerable amount of computational resources required has been provided by the Jülich Supercomputing Centre at Forschungszentrum Jülich.

Energy and dislocation densities, both in terms of geometrically necessary and total dislocations, are measured in sub-volumes of varying size in unloaded crystals. By this approach, it is possible to obtain several thousand samples, with dislocation densities varying by four orders of magnitude. No fundamental difference has been observed in the contribution of free energies of the total and the GND density. A squared contribution of the GND density that is proposed in some Crystal Plasticity models could thus not be supported. However, it became apparent that the energy is scaling logarithmically with the diameter of sub-volume, or logarithmically with the grain size. This observation agrees with the classical dislocation theory and is attributed to the long range stress fields of dislocations.

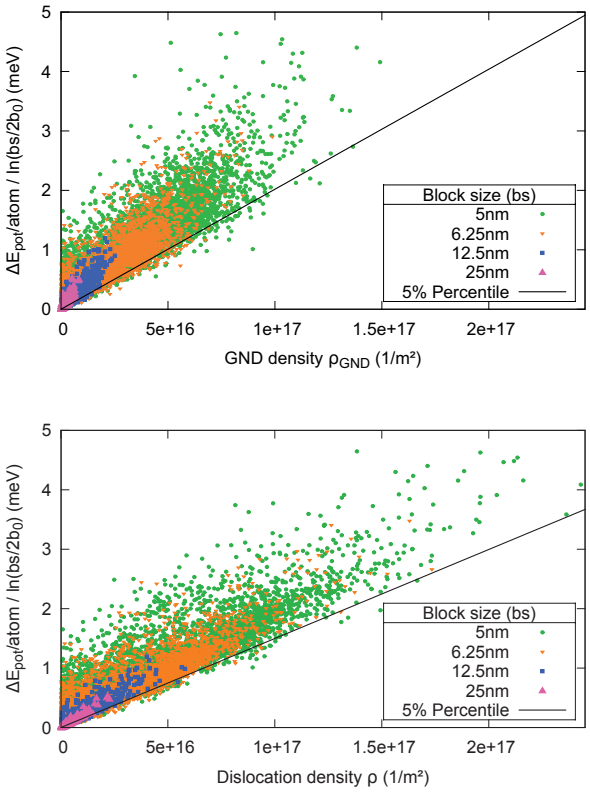


Fig. 7.2: Relationship between the GND density (top) and the total dislocation density (bottom) to the free energy. Although values show scatter, especially for small volumes, the lower limit is following the linear trend once a logarithmic correction term for the sample size is applied.

A related project is considering the influence of carbon on the dislocation mobility in bcc-Fe, which is an interesting phenomenon in static strain aging. Dislocation mobility and carbon diffusion take place at different time scales. In order to overcome the long-time scales of diffusion, a coupled approach of molecular dynamics (MD) and Monte Carlo (MC) was developed.

Some efficient sampling scheme is inevitable to identify possible diffusion sites. First-principles studies claim octahedral sites to be energetically favourable locations for light elements like carbon. Therefore, bcc-Fe bulk is modelled after marking all octahedral sites. Dislocations could be introduced in the crystal along with placeholders, acting as virtual particles.

A Metropolis MC algorithm is implemented to sample carbon diffusion by appropriate trial moves on randomly selected placeholders. A sphere is constructed around a tagged particle with a radius, beyond which the influence of a trial move is negligibly small. The trial moves are either accepted or rejected with a probability of the corresponding statistical ensemble. Trial moves include the switching of a placeholder into carbon, carbon into a placeholder, or changing position of carbon atoms. Trial moves ensure equal probability for visiting all phase space configurations, hence detailed balance is satisfied.

Parallel sampling is done by non-interacting moving blocks on concurrent CPU domains. A moving block position is randomly selected and a trial move is performed. In case of acceptance, neighbouring CPUs are chosen as per block position and changes in configurations are updated by MPI communications.

Relaxation of a new configuration with diffused carbon is continued further with MD simulation steps which allows to study the influence of carbon on dislocation mobility. This approach turns out to have some generality and also allows to study crystals with complex dislocation networks.

To investigate the microstructure formation mechanisms in coating layers during the spraying process of hot nano-particles onto a cooling substrate, large-scale MD simulations were conducted. For a realistic modelling of microstructure, both the nano-particles and the substrate were modelled on the atomistic level, where interactions were computed within the embedded atom model. To evaluate the influence of processing parameters on the morphology of the coating structure, simulations with varying parameters, including initial temperature, size, and velocity of the sprayed particles were conducted.

In the case of metallic coatings, copper particles with sizes of 10 nm to 30 nm were used for spray materials. The final microstructure of the coating is a result of the effects of melting, solidification and elastic and plastic deformation during individual impact as well as the influence of many consecutive impacts. If the sprayed particles are molten, conformal contact areas between substrate and coating are formed, which leads to high densities and low defect concentrations that provide good thermal conductivity. As a result, the final coating structure can be expected to show no formation of large pores. Such pores can be observed, however, in the case of particles that have been plastically deformed without being fully molten. These particles create a "shadow region" for subsequent particles and form more irregular surface structures leading to coatings with more porous microstructures. A thermodynamic model was developed which confirms the trend observed from MD calculations.

Relevant for thermal barrier coatings are ceramic layers. In large scale MD simulations, YSZ (Yttria (w.t. 8% Y_2O_3) stabilized Zirconia) particles, with size up to 100 nm, were simulated to investigate the dependence of ceramic coating structures on the processing parameters. For spray velocities increased from 0.5 km/s up to 2.0 km/s, different layer structures are to be expected, ranging from simple mechanical deformation to melting/solidification (ductile) transitions and a transition regime in between where crack nucleation (brittle) is observed. Such results provide information on the basic mechanisms involved during the thermal spraying process and help to interpret and predict structure formation in coatings under different experimental conditions.

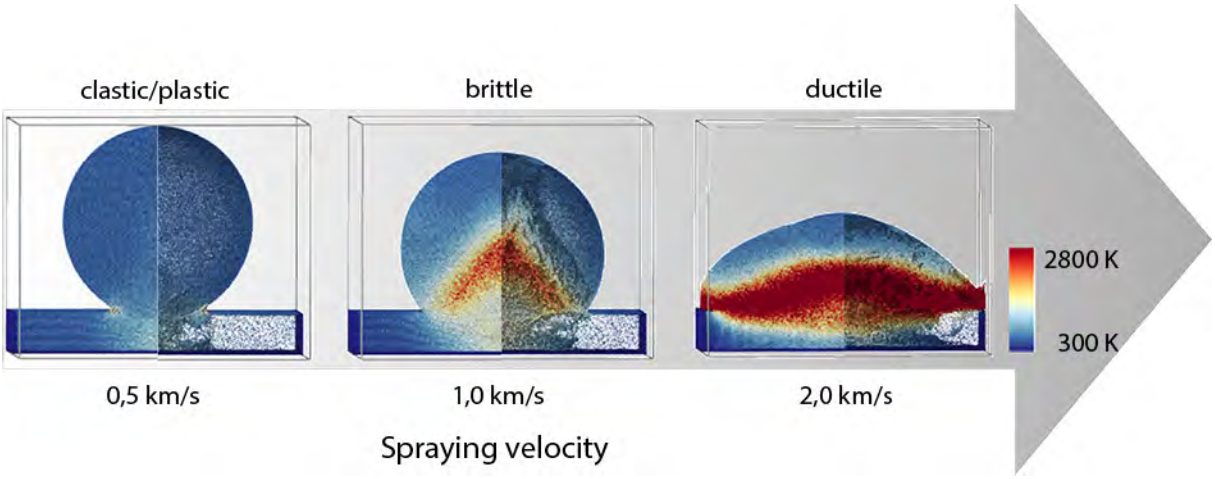


Fig. 7.3: Structural changes in YSZ for nano-particles of 100 nm diameter and an initial velocity ranging between 0.5 km/s and 2.0 km/s.

Structure formation on a mesoscopic length scale cannot be investigated by atomistic methods any more. On these scales, the phase-field method is an established technique for investigations of microstructure evolution during materials processing. In multiphase field simulations, grains of different phases and orientations called phase fields, are represented by auxiliary functions forming and partition of unity and provide an interface between grains of finite size. The phase-field equations only have to be solved at this diffuse interface. Solving the phase-filed equations on a parallel computer can lead to load imbalances, i.e., the work is unevenly distributed over the processors which results in a loss of computational efficiency. A distributed memory parallelization for the multiphase field library OpenPhase has been developed that takes these load imbalances into account and provides techniques to balance the computational load efficiently. The com-

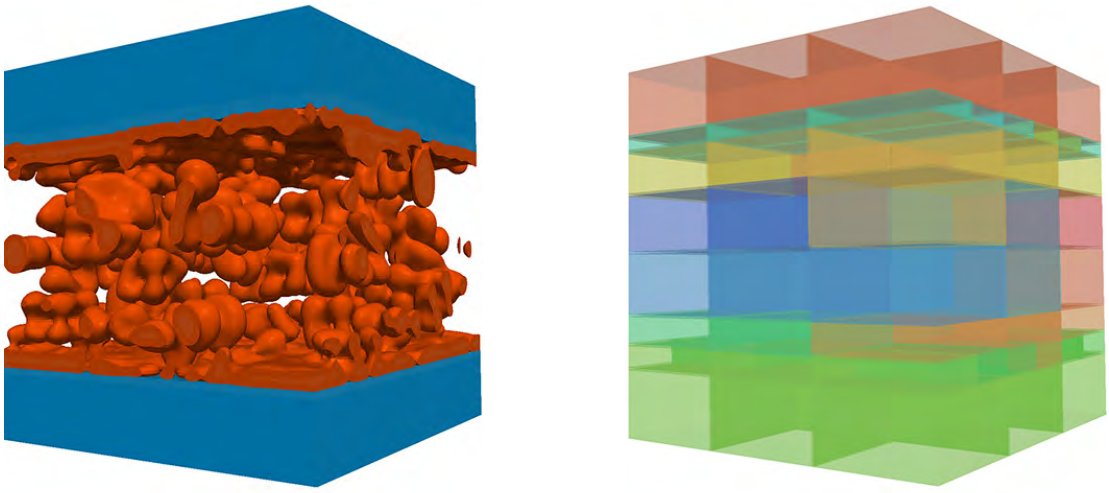


Fig. 7.4: Benchmark simulation of eutectic solidification in an a-phase channel (left) and the block structure of parallel work distribution, where the colour indicates the ranks of the processes assigned to these blocks (right).

putational domain is divided into several rectangular blocks, generally more than the number of MPI processes. To avoid unnecessary synchronization between processors during one time step, a wide halo approach is used. Blocks are assigned by a greedy graph partitioning heuristic that tries to minimize communication and the maximum load among the processes. This heuristic gives an upper bound for the maximum load imbalance depending on the block with the highest computational load. Recursive bisection aims at reducing the maximum load to achieve a better upper bound. Splitting a block, however, introduces an additional computational as well as communication overhead. A criterion for bisection of blocks has been derived and implemented.

The code has been benchmarked in several small test cases to give correct results and has been applied to realistic problems such as Mg-Al-solidification. It is found that load balancing can significantly improve performance especially when combined with hybrid parallelism, thus reducing the overhead created by the wide halo. *Fig. 7.4* shows a simulation of secondary nucleation in a channel between magnesium-rich dendrites and depicts blocks and their assignment to processes. The parallel version of OpenPhase makes three-dimensional large-scale simulations viable that were previously impracticable due to memory limitations and excessive execution times.

Advanced Study Group Modelling

8. Advanced Study Group Modelling

Prof. Dr. Jörg Neugebauer
Dr. Tilmann Hickel
Dr. Robert Spatschek

The objective of the Advanced Study Group (ASG) Modelling is the development, implementation, and application of quantum mechanical based simulation techniques to reliably predict properties and mechanisms in modern engineering materials. It serves as a centre of competence for different concepts in materials modelling, supporting the research at ICAMS in particular at the most fundamental scale which is dominated by electronic interactions and individual atomic processes. Most of the research activities of the ASG are situated in the department of Computational Materials Design of the Max-Planck-Institut für Eisenforschung, headed by Prof. Jörg Neugebauer.

A driving force for all projects in the ASG is the fact that the inherent complexity of engineering materials renders any direct brute force quantum mechanical approach unfeasible. Therefore, well-controlled approximations and efficient numerical formulations are of utmost importance, both at the quantum mechanical level as well as for bridging the gap between the electronic/atomistic and the higher scales considered by the ASG and other departments of ICAMS. The integration of the ASG happens via various joint projects that have been continued or newly initiated in 2014 and have resulted into several publications together with partners at ICAMS. In general, the ASG follows four major research routes:

Analyzing and improving the accuracy of ab initio techniques

Within 2014 the ab initio calculation of thermodynamic materials properties continued to be a key topic for the ASG in 2014. This involves several aspects, such as the crystalline phases, lambda (i.e., magnetic) transitions, point defects and strain dependence. Many of the developed concepts have also entered the set of publications that resulted from the Ringberg unary workshop 2013, jointly organized by the Department STKS (Suzana G. Fries) and this ASG (Tilmann Hickel), and which have been published in January 2014. Here, only two highlights shall be briefly mentioned.

On the one hand, the understanding of the interplay of magnetic and vibrational degrees of freedom in Fe-based materials has substantially improved (Fritz Körmann). The previously developed spin-space averaging (SSA) technique has already given access to atomic forces well above the Curie temperature. However, the description of phonons in the vicinity of the critical temperature where the ferromagnetic long-range order (LRO) is broken or where the paramagnetic (PM) disorder is affected by short-range ordering (SRO) was still unresolved (*Fig. 8.1*). We have now been able to overcome this shortcoming by a novel interpolation scheme that incorporates spin quantum Monte-Carlo simulations for the magnetic energy. These results compare well with and explain state-of-the-art temperature-dependent phonon measurements, which have been performed by the group of Brent Fultz (Caltech, USA).

On the other hand, we have achieved a breakthrough in the understanding of anharmonic lattice vibrations (Albert Glensk, Blazey Grabowski). Here, the key observation was that the anharmonic entropy of the macroscopic system, which is very hard to calculate, can be traced back to the local anharmonicity (LA) of pairwise atomic interactions, a quantity that can be computed more easily. Using this insight, we were able to derive and benchmark a highly efficient approach which now allows us to compute anharmonic free energy contributions using only a few T=0 K rather than expensive molecular dynamics DFT calculations.

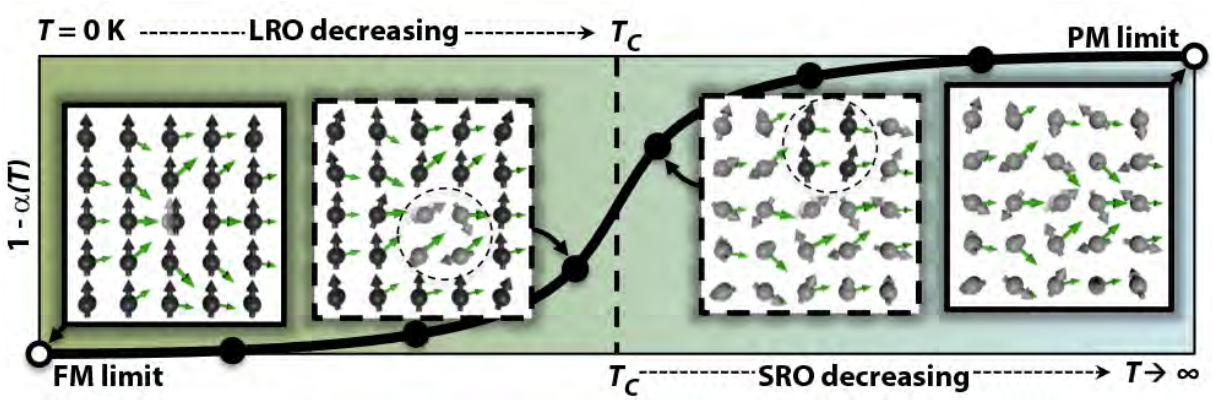


Fig. 8.1: Sketch of the novel approach to treat magnetic disorder. It allows to go beyond the conventionally employed adiabatic approximation by coupling the energetics of the magnetic system with explicit DFT force constant calculations (displaced spin in the middle of each sketch). The gray and green arrows indicate the local magnetic spins for each atom and the interatomic forces (restoring forces when displacing the center atom), respectively. The explicit force constant calculations are carried out for the two limits of completely ordered (left side) and fully disordered spins (right side). The force constants for the intermediate temperature regime (dashed squares) are obtained by coupling the two limits with quantum Monte Carlo simulations for the magnetic subsystem which explicitly include long- and short-range-order effects.

Connecting the quantum-mechanical to engineering scales

While quantum-mechanical calculations provide an important first step in the multiscale hierarchy, calculations of relevant properties on the engineering scale require in most cases additional simulation techniques. Therefore, the ASG Modelling continued to extend and improve the multi-scale program packages S/PHI/nX (Christoph Freysoldt) and Pylron (formerly pyCMW). The latter became an increasingly valuable tool to generate, manage, analyse, and visualize huge amounts of data from various electronic and atomistic simulations in 2014 and is currently shared with the Department AMS (Thomas Schablitzki).

Methodologically, the connection to the engineering scales is achieved by larger scale simulations with empirical potentials (grain boundary motion or particle-dislocation interaction), by kinetic Monte-Carlo simulations (TTT diagrams of precipitate formation), or by Green's functions approaches (to capture long-range elastic fields). In 2014 a particular focus was the understanding of the role of carbon in microstructure features of steels. This involves, for example, the redistribution of C during the phase transformation from austenite to martensite during cooling (Xie Zhang). The investigations revealed the presence of an intermediated structure interconnecting the crystal structures of austenite on the one side and ferrite and cementite on the other side. This structure intrinsically contains the required nucleation sites for an accumulation of carbon.

If stacking faults are formed in austenitic steels, the opposite mechanism of a carbon depletion is observed. Because the HCP-like atomic configuration in the centre of an intrinsic stacking fault is energetically unfavourable for C, it experiences a strong driving force to escape into the FCC matrix. This process is kinetically suppressed at room temperature, but the energetic barriers can be overcome by C if the thermal energy is sufficiently large (*Fig. 8.2*).
A deeper analysis of this anti-Suzuki effect allowed us to explain experimental differences in stacking-fault energies by connecting the mobility of C with the experimental boundary conditions.

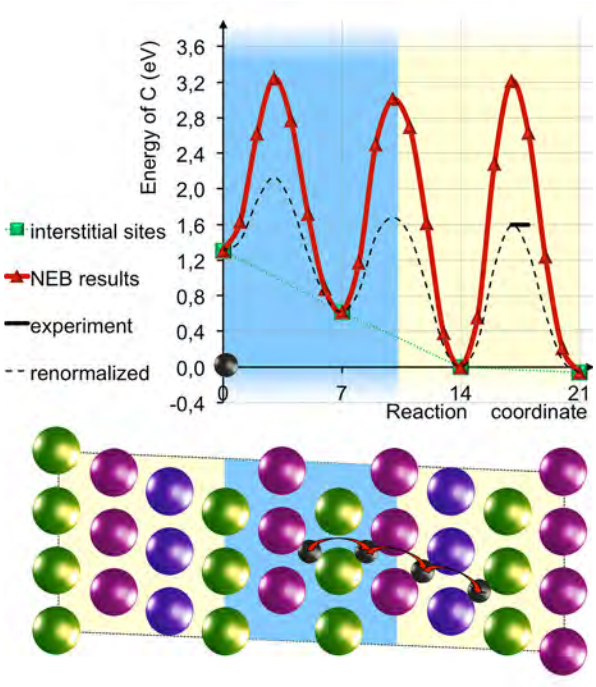


Fig. 8.2: The energetics of a single carbon atom along a diffusion path from the centre of an intrinsic stacking fault into the matrix. The differently shaded areas indicate the HCP (centre of stacking fault) and FCC stacking sequence. The green square symbols (connected by a dotted line as a guide for the eye) provide the C solution enthalpies in the interstitial sites, whereas the red solid line represents the energy barrier for the diffusion. The black, dashed line visualises an energy profile obtained after renormalising the ab initio values to match the experimental value in the bulk FCC region.

Translating industry-relevant materials science questions into formulations accessible by ab initio methods

Following the concepts of integrated computational materials engineering (ICME), the ASG Modelling has always had the aspiration to perform research that yields an improvement of materials for industrial applications. Therefore, the ASG has been continuously seeking an exchange with industrial and experimental partners within and beyond ICAMS. In this context, hydrogen embrittlement continued to be a central field of research for the group. Major topics were the trapping of hydrogen at interfaces between kappa carbides and the steel matrix (Poulumi Dey) as well as the interaction of hydrogen with dislocations (Gerard Leyson).

Similarly, the group continued its studies of advanced structural materials such as high-Mn steels within the SFB761 "Stahl – ab initio". Within this consortium, crash-box experiments have been performed recently in order to understand the deformation behaviour under extreme conditions. The crashworthiness of twinning-induced plasticity (TWIP) steel is intrinsically related to the strain hardening, which can best be captured with crystal-plasticity methods that use dislocation density-based constitutive models (Franz Roters, MPIE). The relevance of dislocation twinning for the overall hardening behaviour, however, sensitively depends on the stacking fault energy (SFE) of the steel. This parameter is accessible to ab initio calculations, though details of its dependence on temperature and magnetism are still subject to investigations within the ASG (Ivan Bleskov). The SFE can also be determined within the CALPHAD approach, which does not take the atomistic character of a stacking fault into account and contains inaccessible parameters like the interface energy. The latter, which so far could not be experimentally determined, is often considered as an empirical constant of 10 mJ/m2 for high-Mn steels. In contrast to this, ab initio calculations are based on quantum mechanical principles and therefore enable us to systematically consider and investigate the physical nature and chemical dependence of this parameter. This knowledge made a substantial contribution to multi-scale simulation of the deformation behaviour of the crash-box.

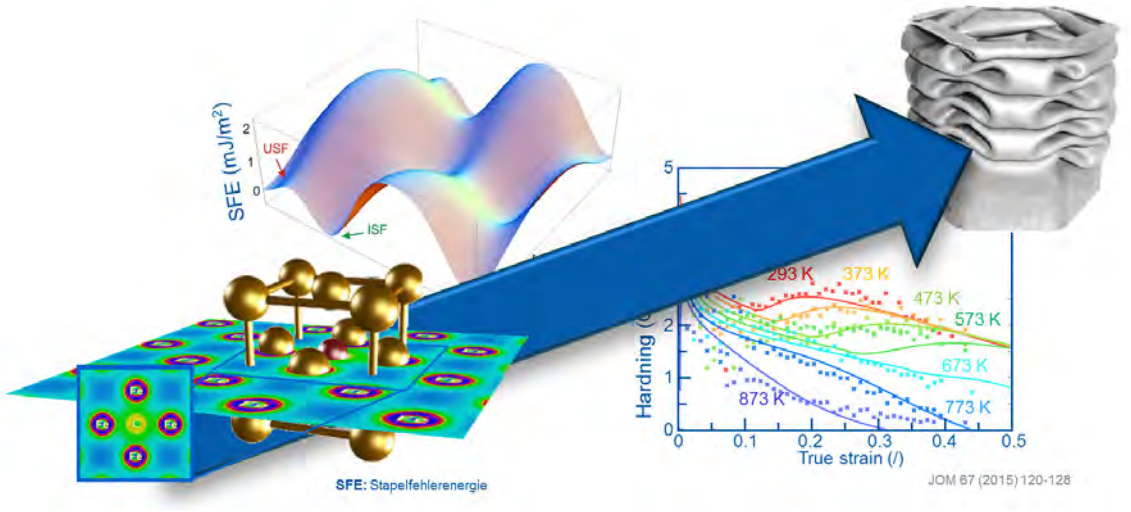


Fig. 8.3: Three-level ICME approach for crash worthiness assessment. Level 1: ab initio calculation of electronic structure, Level 2: Identification of a key ab initio parameter for the hardening behaviour – the stacking fault energy, Level 3: Constitutive models to be used in FEM simulations.

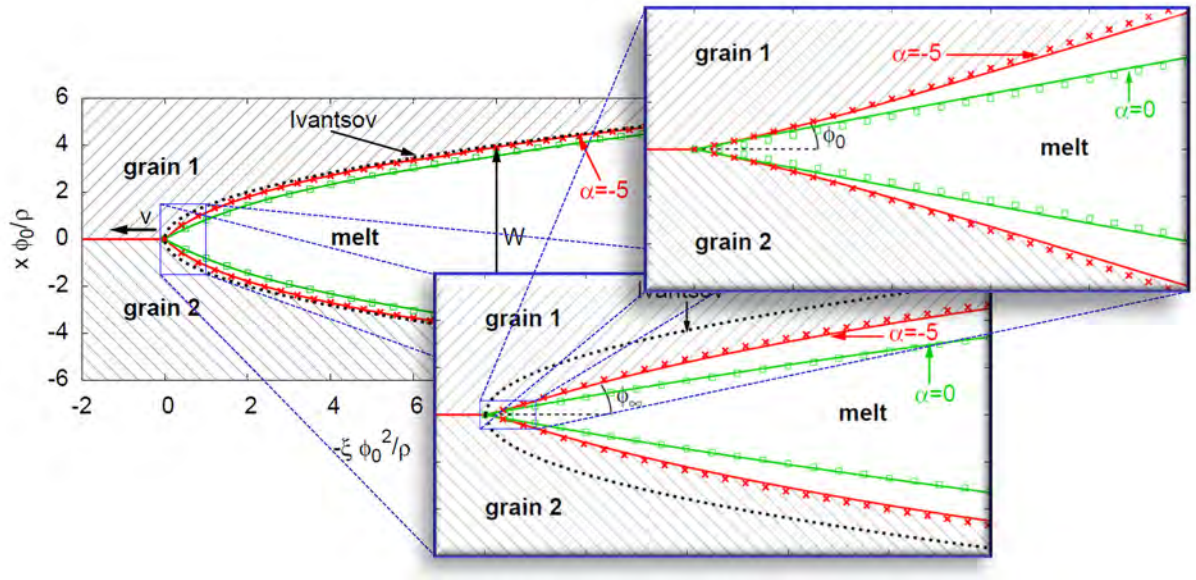


Fig. 8.4: Melting along a dry and overheated low angle grain boundary. The melt front propagates from the right to the left. On the largest scale (micrometer) the melt finger is parabolic far behind the triple junction of the two solid grains and the melt. On intermediate scales, a finite mesoscopic contact angle ϕ_∞ is formed. On the nanometer scale, short ranged structural interactions between nearby solid-melt interfaces lead to a bending of the interfaces. As a result, the microscopic contact angle ϕ_0 deviates from the mesoscopic dihedral angle ϕ_∞. The steady state velocity of the melting process is strongly influenced by the short ranged interaction due to the overlap of nearby solid-melt interfaces.

Materials modelling on the mesoscale

Some activities in the ASG Modelling are devoted to the understanding of phenomena appearing on dimensions between the atomic and continuum scales (Robert Spatschek). For this purpose, various computational and analytical techniques, particularly tailored to different applications, are developed and used.

In this context, a major part of the research in 2014 was devoted to melting along grain boundaries. In a recent study, a nano-mesoscale description in terms of a sharp interface model and a phase-field description have been performed to capture the wide range of involved length scales. It was the aim of this work to predict the growth velocity and the length scale that describe the pattern (*Fig. 8.4*). Specifically, we obtain analytic and numerical solutions that are influenced by structural disjoining forces in the experimentally relevant regime of small deviations from the melting temperature (Claas Hüter, Pavan Kumar Bhogireddy, Oleg Shchyglo).

A multiscale approach is employed within the ASG in order to improve the understanding of hydrogen embrittlement in steels. Here, our group focuses on mesoscale simulations that can be based on ab initio input and allow the prediction of hydride formation next to dislocations, interfaces, or surfaces. The ASG combines, for this purpose, thermodynamics, elasticity theory, and finite element simulations. Furthermore, aspects of fracture mechanics and phase-field methods are used to predict hydrogen-inducted crack formation and propagation.

Advanced Study Group Input Data and Validation

9. Advanced Study Group Input Data and Validation

Prof. Dr.-Ing. Gunther Eggeler
Dr.-Ing. Jan Frenzel
Junior-Professor Victoria Yardley

In 2014, the ASG Input Data and Validation made significant progress in the field of Ni-Ti-based shape memory alloys. Depending on composition, Ni-Ti can exhibit a thermal or a mechanical memory. Shape memory alloys represent a fascinating class of materials since they can recover their initial shape after a large deformation during heating or unloading after straining. Today, shape memory alloys are used for special engineering applications such as actuators, circuit breakers, pipe couplings, etc. They are also important materials for flexible medical products such as vascular stents, guide wires, blood filters and special surgical instruments.

The shape memory effect relies on a martensitic transformation, a diffusionless transformation which occurs in the solid state. In the case of Ni-Ti, phase transformation temperatures strongly depend on the Ni concentration (*Fig. 9.1 a*). Materials scientists have struggled to explain this relation since 1965, when Wang, Buehler and Pickard first described the strong dependence of the martensite start temperature M_S on the Ni concentration in near-stoichiometric binary Ni-Ti alloys. In our work, we used differential scanning calorimetry and density functional theory (DFT) simulations to rationalize these findings. As a new result, it was observed that the martensite start temperature strongly depends on the heat of transformation ΔH. Together with Ingo Opahle and Ralf Drautz from the Department AMS, we have shown that ΔH decreases as the Ni concentration increases from 50.0

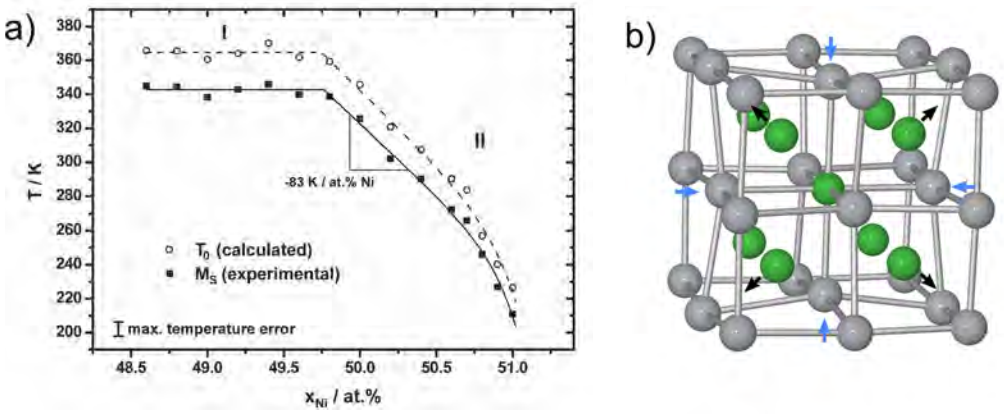


Fig. 9.1: Effects of alloy composition in binary Ni-Ti shape memory alloys (copyright Elsevier). a) Dependence of the martensite start temperature M_S on Ni-concentration. b) Visualization of local lattice relaxation around a Ni(Ti) antisite defect.

to 51.2 at.%. This causes a shift in the Gibbs free enthalpy difference of austenite $G_A(T)$ and martensite $G_M(T)$, which in turn results in a lower martensite start temperature. Our DFT results suggest that the strong decrease of ΔH is caused by a stabilization of the high-temperature austenite phase by structural relaxations around Ni antisite atoms, together with a gradual destabilization of the low- temperature martensite phase. *Fig. 9.1 b* shows lattice relaxation around an antisite defect in a Ni-rich Ni-Ti shape memory alloy. Our results contribute to a better understanding of shape memory alloys. They are also relevant for the design of new shape memory alloys with improved functional properties. Our work has recently been accepted for publication in Acta Materialia.

Another main focus of our work in 2014 was the investigation of the process of martensitic microstructure formation in ferrous alloys. This work complements the phase-field-based methods being developed in the context of the ICAMS Demonstrator Project for the simulation of martensitic microstructures. The effect of nickel content on the M_S temperature and microstructure in the Fe-Ni binary system in the range 20-32.5 at.% Ni was investigated. A monotonic decrease of M_S from around 200 °C to cryogenic temperatures with increasing Ni content was accompanied by a transition from a parallel, lath-type microstructure (*Fig. 9.2 a*) to a microstructure containing plates of varying sizes with triangular regions of retained austenite between plates (*Fig. 9.2 b*). Further ex-

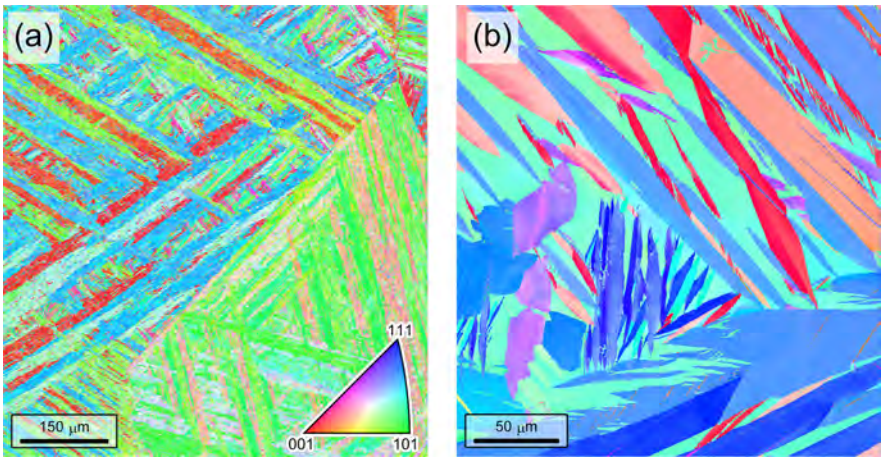


Fig. 9.2: Electron backscatter diffraction inverse pole figure images of microstructures in Fe-Ni binary alloys. (a) Lath-type microstructure in Fe-25 at.% Ni alloy; (b) Plate-type microstructure in Fe-32.5 at.% Ni alloy.

periments to investigate the composition region over which the transition from lath to plate microstructure takes place are currently in progress.

In a martensitic transformation, a single grain of the parent austenite phase subdivides into martensite crystallites with different orientations (martensite variants) according to a crystallographic orientation relationship between the austenite and martensite. These different orientations appear as different colours in the inverse pole figure orientation maps shown in *Fig. 9.2*, which were obtained using electron backscatter diffraction (EBSD).

The characteristics of the variant orientations in the Fe-Ni alloy microstructures were investigated. It was found that in both plate and lath microstructures, specific misorientation relationships between neighbouring variants are preferred. In addition, a certain amount of scatter in the variant orientations was observed, the degree of this scatter increasing with increasing M_S temperature. The results of the Fe-Ni study were presented by Pascal Thome at the ICOMAT conference in Bilbao, Spain in July 2014.

The above results, together with previously acquired data from step-by-step studies on the growth mechanisms of plate martensite, already give important hints about the mechanism of the transformation at different temperatures, and it is hoped that the ongoing work on alloys in the transition region and on transformation energetics under different cooling rates will bring more comprehensive insight that can inform the development of the phase-field models for martensite formation.

In order to perform more detailed analyse of microstructures in martensitic and tempered martensitic microstructures than is possible using commercially available EBSD analysis software, we have also extensively focused our efforts on algorithm development using the open-source crystallographic analysis toolbox MTEX for MATLAB (http://mtex-toolbox.github.io/). Our paper on the development and application of algorithms for use in the characterisation of scatter in martensite variant orientations was published in Materials Science and Technology in September 2014. *Fig. 9.3*, one of the illustrations from this paper, demonstrates that the orientational variation seen within a single martensite block or plate is not randomly distributed, but instead changes gradually and continuously with position. We believe that these orientation variations are associated with the accommodation of shape strains within the martensite.

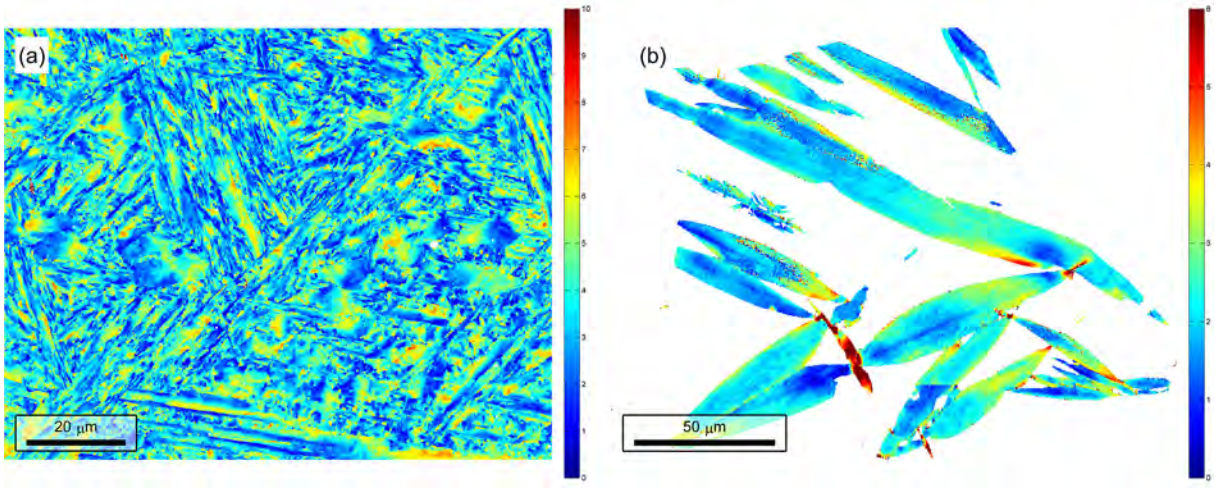


Fig. 9.3: (a) Deviation of local variant orientation from ideal Kurdjumov-Sachs orientation relationship in the tempered martensite ferritic creep-resistant steel FV535; (b) deviation of local variant orientation from ideal Nishiyama-Wassermann orientation in Fe-30 at.% Ni binary alloy (copyright Maney).

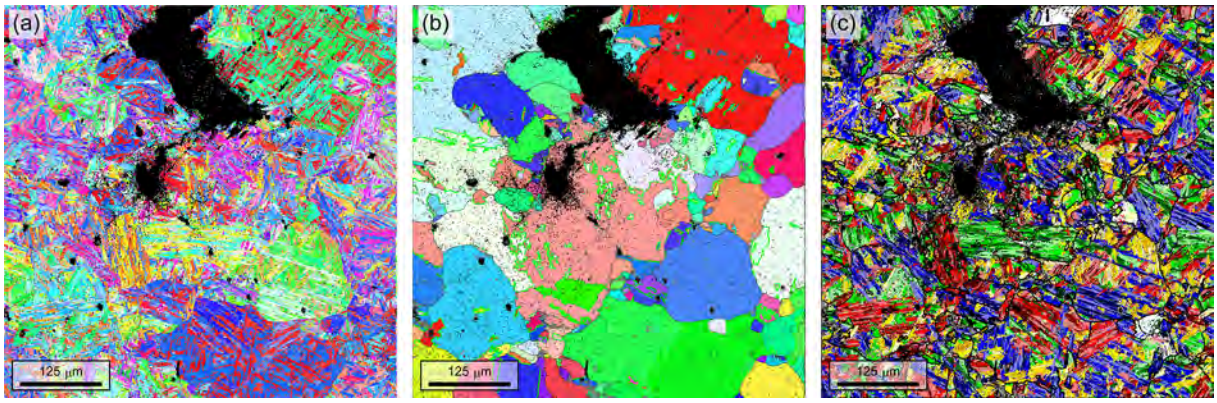


Fig. 9.4: Microstructures in the vicinity of a creep crack in a crack growth test specimen of the tempered martensite ferritic heat-resistant steel X20CrMoV12-1: (a) tempered martensitic microstructure; (b) reconstructed prior austenite microstructure; (c) block and packet microstructure. In all images, black regions represent voids and cracks. (Mechanical testing and EBSD data acquisition by Shirin Fahimi).

A second paper, on an algorithm for the reconstruction of prior austenite grain microstructures and its application to the identification of crack and cavitation sites in terms of the features of tempered martensite microstructures (prior austenite grains, packets and blocks), appeared in the March 2015 issue of Materials Science and Technology. *Fig. 9.4* shows an example of the application of this algorithm to the area around a creep crack tip in a compact tension crack growth test specimen. In *Fig. 9.4 (a)*, the inverse pole figure orientation map for the tempered martensite can be seen, with the void and crack regions of the sample shown in black. The calculated prior austenite grain microstructure can be seen in *Fig. 9.4 (b)*. It is clear from the differences in colour, which represent differences in crystal orientation, that the widest part of the crack runs along a prior austenite grain boundary, whereas the tip of the crack penetrates into a single prior austenite grain. Twin boundaries, which are relatively common in austenitic iron, are shown in green in *Fig. 9.4 (b)*, and general grain boundaries in black. The martensitic substructure can be seen in *Fig. 9.4 (c)*. Areas of the same colour (blue, red, yellow or green) within a single prior austenite grain represent martensitic packets, and the different shades within these represent martensite blocks. An image of this type enables us to determine whether those voids that can be seen from *Fig. 9.4 (b)* to be within prior austenite grains are located on block or packet boundaries. Systematic studies of the effect of test temperature on void and crack sites are currently underway.

In addition to its application in understanding damage formation, the reconstruction algorithm is also being used for more fundamental studies of the effect of carbon content and heat-treatment parameters on block and packet sizes in the context of the ICAMS Demonstrator Project.

The ASG Input Data and Validation has recently organised an MTEX EBSD analysis workshop for researchers and students that dealt with common tasks in the analysis of martensitic and other microstructures. Research projects involving detailed analyse of experimental and simulated microstructures have been or are carried out by students from the Materials Science and Simulation (MSS) course. The images in *Fig. 9.5* are taken from the work of MSS student Huzaifa Shabbir. An initial microstructural model is constructed to mimic important features of a tempered martensite ferritic microstructure. After meshing and a simulated tensile test using crystal-plasticity finite element modelling in ABAQUS, the resulting changes in morphology and crystal orientation can be investigated with MTEX. This procedure allows easy comparison between the texture and misorientation distribution developed during the simulated test and those developed experimentally.

Fig. 9.5: Orientation images of model tempered martensite microstructure subjected to simulated uniaxial tensile test: (a) before test; (b) 25% strain; (c) 75% strain; (d) 100% strain. Images from Huzaifa Shabbir.

Advanced Study Group Processing and Characterization

10. Advanced Study Group Processing and Characterization

Prof. Dr. Wolfgang Bleck
Dr. Ulrich Prahl
Dr. Sebastian Münstermann
Alexandros Serafeim
Mohamed Sharaf
Wenwen Song
Napat Vajragupta

The Advanced Study Group "Processing and Characterization" at the Steel Institute (IEHK) at the RWTH Aachen aims at modern materials characterization, integrative numerical simulation of materials, materials processing, and modelling of failure at different length scales in steels and components. The ultimate goal is to deepen the knowledge on physical, mechanical, and microstructural mechanisms in steels in order to enable improvement of their properties by means of the tailored microstructure design and also to provide the cutting edge solutions for steel production, processing, and application.

By means of the SemiProductSimulationCenter, special steel alloys of industrial quality can be provided on laboratory scale (*Fig. 10.1*). Directly after casting, a hydraulic press is used to deform ingots in a temperature- and deformation-controlled manner. For temperature control and advanced annealing cycles, two electrical furnaces are available. For splitting the process and for a post-treatment quenching operation, an autogenous flame cutter and a water basin are installed. The material properties and their variations at different experimental conditions are then analysed using a variety of microstructural characterization facilities.

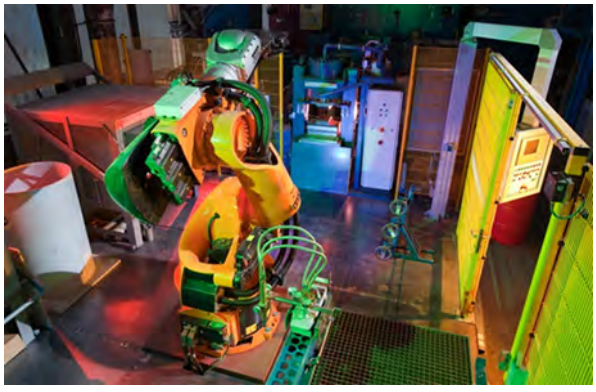


Fig. 10.1: SemiProductSimulationCenter at IEHK

Within the project "Diffusion-controlled bainitic phase transformation", Wenwen Song investigates nano-sized carbide precipitation during bainitic phase transformation at different temperatures in high carbon steel $100Cr_6$ by means of transmission electron microscopy (TEM) and anomalous small-angle X-ray scattering (ASAXS). The precipitation location morphology and size of the nano precipitates were characterized by TEM and provided the basis of the morphological assumptions for anomalous small-angle X-ray scattering (ASAXS) analysis on the types and phase fractions of the nano-carbides. ASAXS was measured at beamline B1 of the synchrotron storage ring DORIS III (DESY, Hamburg). A scattering vector magnitude q range from 0.035 nm^{-1} to 5 nm^{-1} was covered by placing a 2D detector, either Pilatus 1M or Pilatus 300k (Dectris), depending on availability, at two sample-to-detector distances of 883 and 3883 mm. In the ASAXS study, the nano-carbides were distinguished from each other due to the different scattering length densities (ρ(E)) of the different carbides in comparison to iron. The nano-sized carbide precipitation features within the bainitic microstructures at varied temperatures were discussed in terms of thermodynamics and elemental partitioning during bainite formation. We found that the volume fraction of

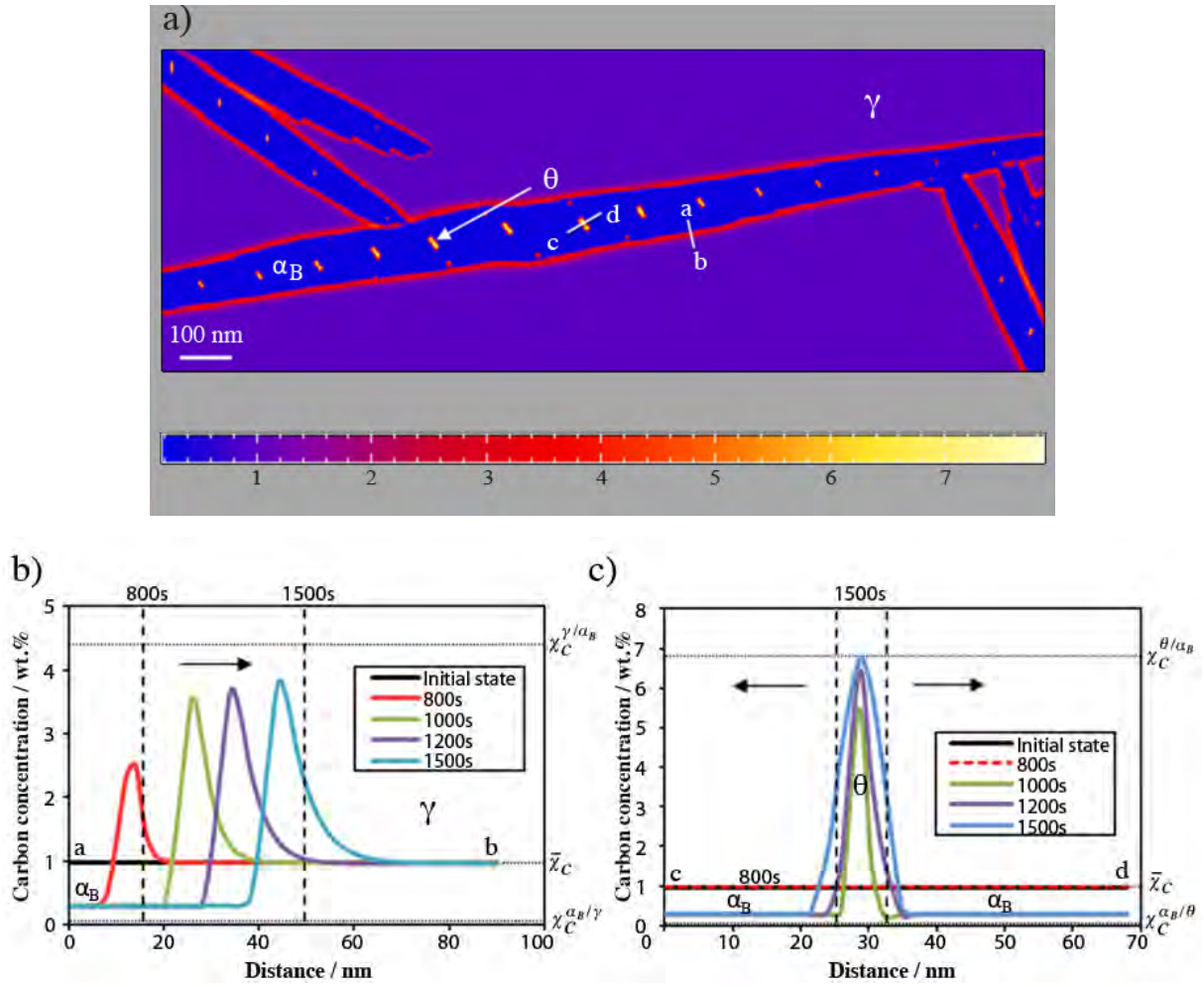


Fig. 10.2: (a) phase-field simulated microstructure in $100Cr_6$ at 260 °C for 1500 s; (b) carbon concentration along a-b line in Fig. 10.2(a) showing the migrating bainitic ferrite/austenite interface and carbon redistribution behaviour during bainitic ferrite thickening in bainite formation at 260 °C in $100Cr_6$; (c) carbon concentration along c-d line in Fig. 10.2(a) showing the migrating bainitic ferrite/cementite interface and carbon redistribution behaviour during cementite precipitation in bainite formation at 260 °C in $100Cr_6$.

θ-carbide in upper bainite at 500 °C is 10 vol.% higher than that in lower bainite at 260 °C, so that we infer that θ-carbide precipitation is more favoured in upper bainite than in lower bainite. However, ε-carbide (Fe2.4C) is more prone to precipitation from lower bainite at 260 °C than from upper bainite at 500 °C. Due to the Cr and C elemental partitioning, Cr carbide may precipitate with a small amount within the upper bainite at 500 °C. In addition, the nano-sized carbide precipitation features during bainite formation in high carbon steel $100Cr_6$ were integrated into the phase-field simulations. From the phase-field simulations, the cementite (θ) precipitation in a single lower bainite plate and the corresponding concentration profiles of carbon redistribution at γ/αB and αB/θ interfaces during the bainitic phase transformation at 260 °C in $100Cr_6$ can be investigated (*Fig. 10.2*). With the summarised results, a comprehansive understanding of the nano precipitates within the bainitic microstructure is achieved by a series of advanced characterization methods and simulation approaches.

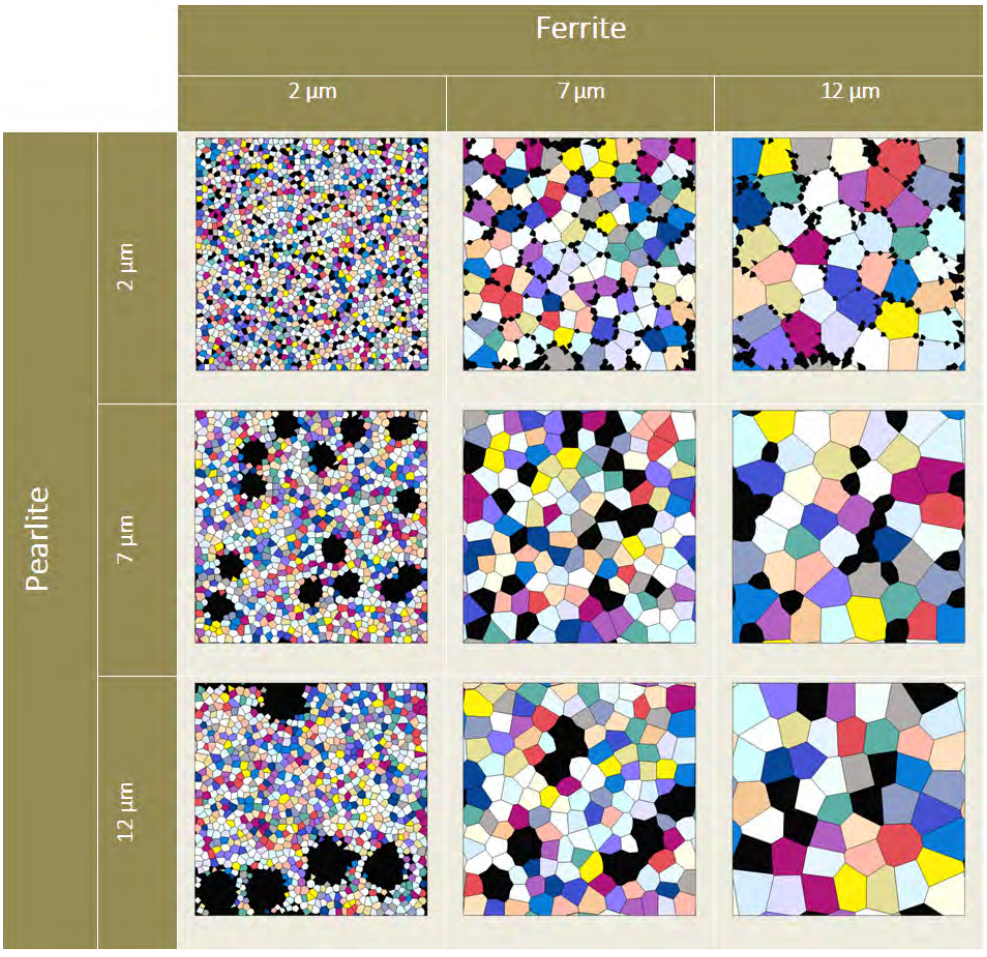


Fig. 10.3: Example SRVEs with a combination of uniform distributions of ferrite grain sizes and pearlite colony sizes. For each of the 9 displayed combinations, 20 instantiations are generated; i.e., a total of 180 SRVEs are exemplarily shown here.

In the project "Effect of microstructure on the growth of short cracks", Mohamed Sharaf investigates the high cycle fatigue lifetime of structural steel components that depends mainly on the phase of fatigue crack initiation and the propagation of microstructural short cracks. A numerical method, which quantitatively describes the influence of microstructural features on the initiation and growth of cyclic microcracks, is developed within the context of microstructure-sensitive modelling. The implementation of kinematic hardening and microdamage on each slip system in a crystal-plasticity model allows for capturing the local accumulation of plastic microdeformation representing slip irreversibility occurring in the crack incubation phase. A load increasing testing technique with continuous temperature measurement, interrupted cyclic bending experiments, and in-situ cyclic tests with the Digital Image Correlation (DIC) technique delivers information about the endurance strength of multiphase steel. By determining local strain distributions and metallographic observation of cyclic microcrack propagation, the experimental basis for the numerical simulations is provided. The material model is implemented in cyclic computations with statistical volume elements (SVEs), which are based on experimental microstructure description using EBSD (*Fig. 10.3*). The extreme value distributions of the resulting accumulation of local dislocation slip are then correlated to the microstructure in an approach to quantify the influence of the distribution of several stereological parameters (phase fraction, grain size, orientation and shape, etc.) on endurance limit and fatigue life in the HCF regime.

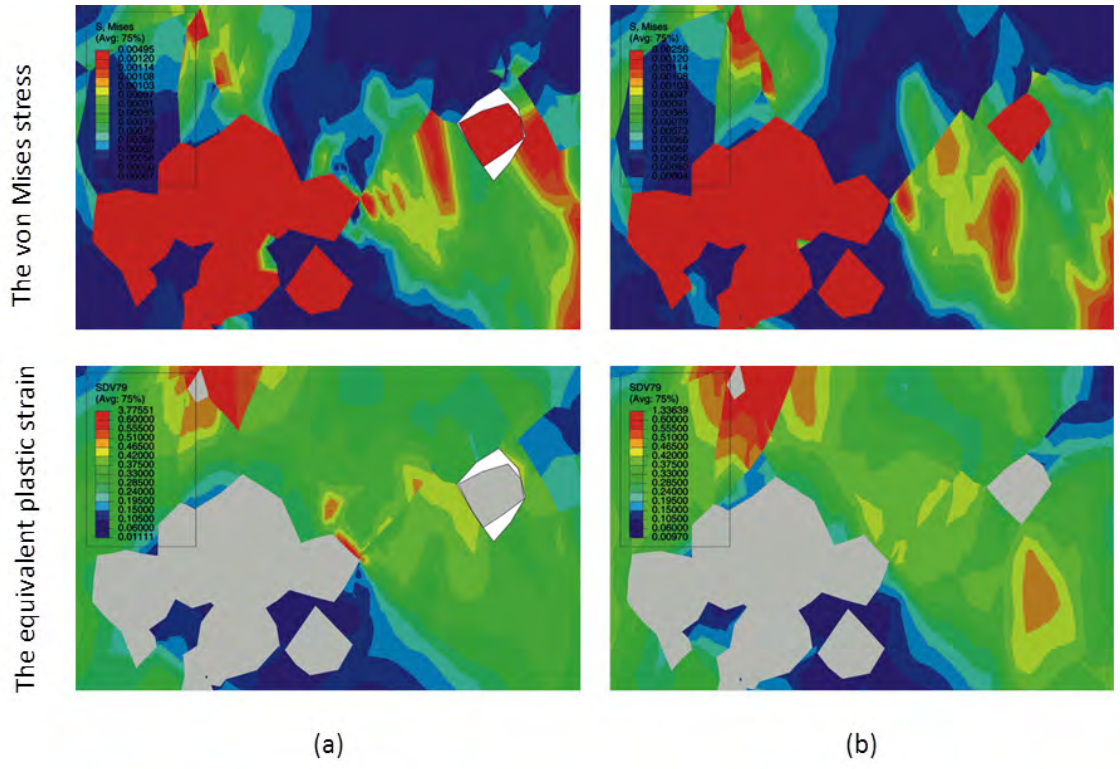


Fig. 10.4: Comparison of the local von Mises stress and equivalent plastic strain distribution between (a) the artificial microstructure model with assigned surface-based cohesive behaviour to the selected phase boundary and (b) the artificial microstructure model without assigned surface-based cohesive behaviour.

In the project "Microstructure based evaluation of real structures in cold formable steels", Napat Vajragupta aims at microscopic scale characterization of failure processes in multiphase sheet steels, like DP and TRIP, and development of the microstructural failure criteria. Within this framework, a modelling scheme to evaluate the influence of microstructure features on microcrack formation has been developed (*Fig. 10.4*). The project covers several work packages like an algorithm to generate the artificial microstructure model, development of the procedure to derive plasticity parameters of constituents, and characterization of the microcrack formation. First, the algorithm to generate the artificial microstructure model was developed. The main target of this work packages was to develop an algorithm to generate a microstructure model that included all the necessary microstructure features, e.g., grain size distribution by utilising the quantitative description of microstructure as input parameters for the weighted Voronoi tessellation algorithm. With the generated microstructure model, the description of constituents' plasticity and the procedure for deriving the parameters were discussed. The crystal-plasticity theory along with parameter calibration by the nanoindentation test and the empirical approach based on local chemical composition and dislocation theory were considered for ferrite and martensite respectively. In order to incorporate the influence of microstructure features on microcrack occurrence in multiphase steel, one of the work packages' aims was to identify microcrack initiation criteria experimentally and numerically. Thus, in situ bending tests to capture the moment of microcrack onset and numerical modelling to determine the adequate criteria were performed (*Fig. 10.4*). By assembling all the work packages, one could investigate the influence of microstructure features on plasticity and damage behaviour via the developed modelling platform proposed in this project.

Advanced Study Group Diffusion and Microstructure Analysis

11. Advanced Study Group Diffusion and Microstructure Analysis

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

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

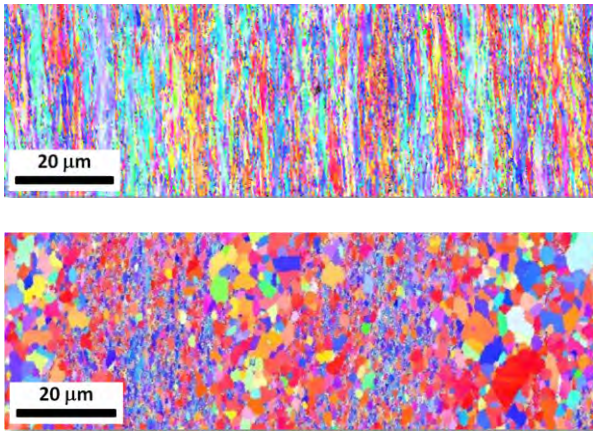


Fig. 11.1: Microstructure of ECAP-processed Ni in the as-prepared state (a), and after annealing at 700 K for 17 hours (b); the Arrhenius plot for the measured self-diffusion coefficients D of 63Ni in ECAP-Ni (c). The Ni diffusion rates in ECAP-processed 99.6 wt% pure Ni (symbols and solid lines) are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

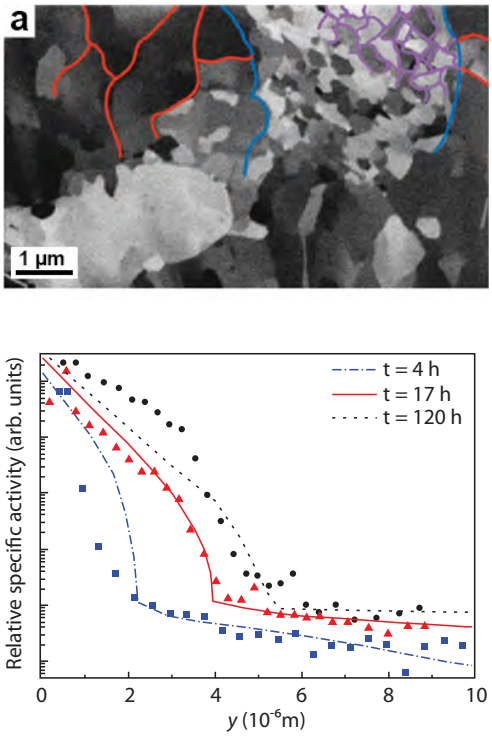


Fig. 11.2: Microstructure and grain boundary types in ECAP-processed Ni in the course of heterogeneous recrystallisation (above) and the penetration profiles of 63Ni as a function of the diffusion time t (left).

Examples for collaboratively addressed topics are:

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

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

ICAMS Members 2014

12. ICAMS Members 2014

Staff at ICAMS

From 2013 to 2014 ICAMS' scientific staff numbers stayed at a constant level. The start-up period ended in 2013, and from the beginning of 2014, 20 positions have been funded by RUB. All remaining positions have been based on third-party funded projects. Fluctuation of scientific staff mainly resulted from the fact that several Postdoc and PhD projects were successfully finished in the last year.

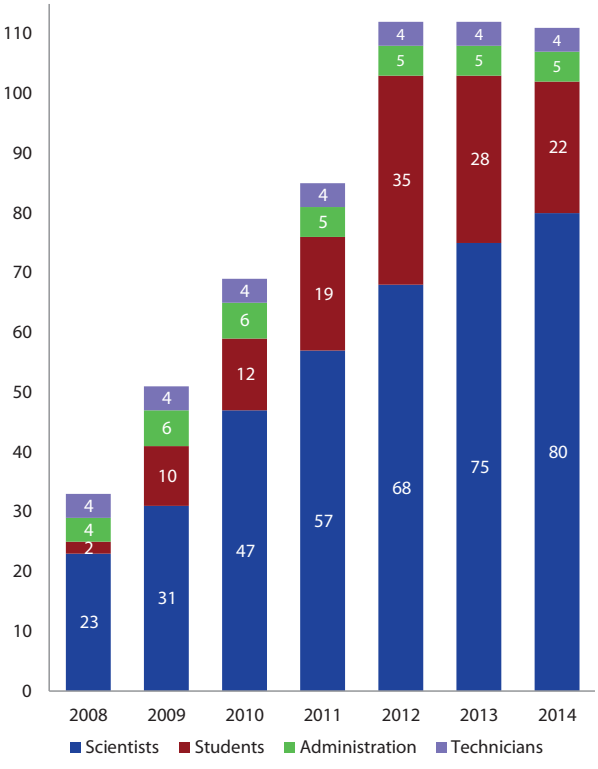


Fig. 14.1: Development of ICAMS staff from 2008 to 2014.

Fig. 14.1 shows the development of ICAMS staff numbers through the first seven years. By the end of 2008 about 30 people were working at ICAMS. From 2009 to 2011 this number increased to more than 60 people, and by the end of 2012 more than 100 people worked at ICAMS, a number which stayed almost constant in 2013 and 2014.

In *Fig. 14.2*, we see that the majority of ICAMS scientists hold a degree in engineering and materials science, followed by degrees in physics, chemistry, mathematics, and computer science. This educational diversity of our research staff provides a fruitful basis for ICAMS' interdisciplinary research.

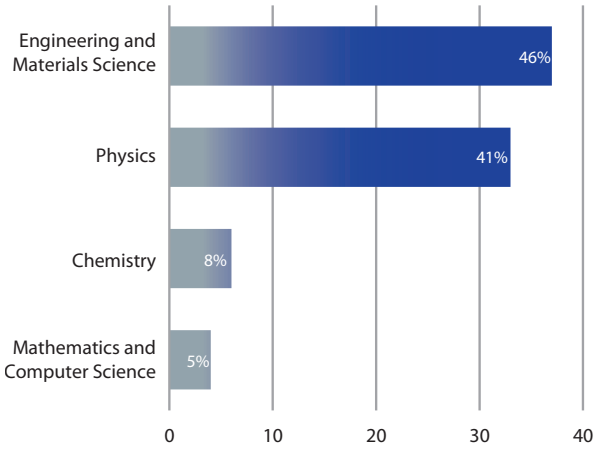
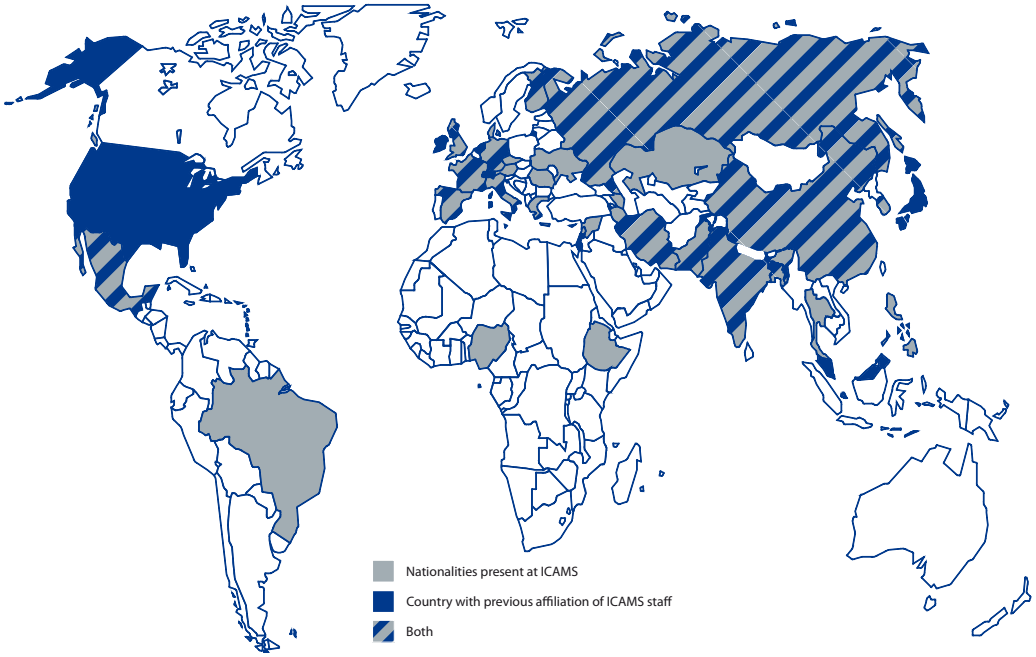


Fig. 14.2: Breakdown of the scholastic background of ICAMS researchers. The educational diversity of the ICAMS research staff provides a fruitful basis for our interdisciplinary research.

In 2014 researchers from more than 20 countries were working at ICAMS (see grey areas in *Fig. 14.3*) and the Advanced Study Groups. 50% of the ICAMS staff is of German and 50% of foreign nationality. For ICAMS, it is of vital importance to attract talented scientists from leading research institutions worldwide. Fig. 3 gives an overview of the countries and institutions the current ICAMS researchers came from to join us. 17 of the 56 institutions are located in Germany, 13 in other EU countries and 26 in non-EU countries. This table demonstrates that ICAMS was able to hire researchers from excellent national and international research institutions. 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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Beihang University, Beijing
Central South University, Changsha
Shanghai University
Chinese Academy of Sciences, Shenyang
Northwestern Polytechnical Univ., Xi'an Shaanxi

Denmark
Aarhus University

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

Finland
University of Helsinki

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Humbolt-Universität, Berlin
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Friedrich-Alexander Univ., Erlangen-Nürnberg
Goethe-Universität, Frankfurt am Main
Albert-Ludwigs-Universität Freiburg
Universität Hamburg
Universität Heidelberg
Forschungszentrum Jülich
Christian-Albrechts-Universität, Kiel
BASF, Ludwigshafen
Universität Stuttgart
Bergische Universität Wuppertal

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Anna University, Chennai
Larson & Toubro Limited, Chennai
Indian Institute of Technology, Guwahati
Indian Institute of Technology, Kanpur
Indian Institute of Technology, Mumbai
Pondicherry University
Indian Institute of Technology, Roorkee

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Shiraz University
Amirkabir University of Technology, Teheran
K. N. Toosi University of Technology, Teheran

Ireland
Trinity College, Dublin

Israel
The Hebrew University, Jerusalem

Italy
NNL of CNR-INFM, Lecce
University of Trento

Japan
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University of Tokio
National Institute for Materials Science, Tsukuba

The Netherlands
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Pakistan
University of Engineering & Technology, Lahore

Philippines
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South Korea
KAIST, Daejeon

Spain
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Switzerland
Swiss Federal Institute of Technology, Lausanne

United Kingdom
University of Oxford
Imperial College, London

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Fig. 14.3: 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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Publications

13. Publications

>> Books and contributions to books

P. S. Engels, C. Begau, S. Gupta, B. Schmaling, A. Ma, A. Hartmaier
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M. Boeff, A. Ma, A. Hartmaier
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Journal of Applied Physics, 116 (2014) 093514

M. Q. Jiang, G. Wilde, J. H. Chen, C. B. Qu, S. Y. Fu, F. Jiang, L. H. Dai
Cryogenic-temperature-induced transition from shear to dilatational failure in metallic glasses
Acta Materialia, 77 (2014) 248-257

J. Millán, S. Sandlöbes, A. Al-Zubi, T. Hickel, P. Choi, J. Neugebauer, D. Ponge, D. Raabe
Designing Heusler nanoprecipitates by elastic misfit stabilization in Fe-Mn maraging steels
Acta Materialia, 76 (2014) 94-105

V. Perekrestov, A. Kornyushchenko, Y. Kosminska, G. Wilde, S. Ostendorp, N. Winkler
Formation of porous low-dimensional nickel systems during near-equilibrium condensation in ultrapure inert environment
Applied Surface Science, 316 (2014) 155-162

U. Tutsch, B. Wolf, S. Wessel, L. Postulka, Y. Tsui, H. O. Jeschke, I. Opahle, T. Saha-Dasgupta, R. Valenti, A. Bruhl, K. Removic-Langer, T. Kretz, H.-W. Lerner, M. Wagner, M. Lang
Evidence of a field-induced Berezinskii-Kosterlitz-Thouless scenario in a two-dimensional spin-dimer system
Nature Communications, 5 (2014) 5169

G. Laplanche, J. Pfetzing-Micklich, G. Eggeler
Sudden stress-induced transformation events during nanoindentation of NiTi shape memory alloys
Acta Materialia, 78 (2014) 144-160

F. Körmann, B. Grabowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, J. Neugebauer
Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment
Physical Review Letters, 113 (2014) 165503

M. Kanani, A. Hartmaier, R. Janisch
Interface properties in lamellar TiAl microstructures from density functional theory
Intermetallics, 54 (2014) 154-163

M. Sharaf, P. Kucharczyk, N. Vajragupta, S. Münstermann, A. Hartmaier, W. Bleck
Modeling the microstructure influence on fatigue life variability in structural steels
Computational Materials Science, 94 (2014) 258-272

N. Vajragupta, P. Wechsuwanmanee, J. Lian, M. Sharaf, S. Münstermann, A. Ma, A. Hartmaier, W. Bleck
The modeling scheme to evaluate the influence of microstructure features on microcrack formation of DP-steel: the artificial microstructure model and its application to predict the strain hardening behavior
Computational Materials Science, 95 (2014) 198-213

A. Zinn, S. Borhani-Haghighi, E. Ventosa, J. Pfetzing-Micklich, N. Wieczorek, W. Schuhmann, A. Ludwig
Mechanical properties of $SiLi_x$ thin films at different stages of electrochemical Li insertion
Physica Status Solidi A, 211 (2014) 2650-2656

L. Klein, A. Zendegani, M. Palumbo, S. G. Fries, S. Virtanen
First approach for thermodynamic modelling of the high temperature oxidation behaviour of ternary γ strengthened Co-Al-W superalloys
Corrosion Science, 89 (2014) 1-5

A. A. Breidi, M. Andasmas, J. C. Crivello, N. J. Dupin, J. M. Joubert
Experimental and computed phase diagrams of the Fe-Re system
Journal of Physics: Condensed Matter, 26 (2014) 485402

S. Schuwalow, J. Rogal, R. Drautz
Vacancy mobility and interaction with transition metal solutes in Ni
Journal of Physics: Condensed Matter, 26 (2014) 485014

>> Theses

A. M. Tahir
Development and validation of a scale-bridging method for simulation of intergranular fracture in body-centered cubic metals
PhD Thesis, Ruhr-Universität Bochum (2014)

B. Reinholz
Discrete disclination dynamics: microstructure evolution in Ni-Mn-Ga shape-memory alloys
PhD Thesis, Ruhr-Universität Bochum (2014)

N. Alemayehu
Intercalation kinetics of battery- and related materials
PhD Thesis, Ruhr-Universität Bochum (2014)

T. Schablitzki
Atomistic study of kinetic processes of solid-state phase transformation in FeCr with topological fingerprints
PhD Thesis, Ruhr-Universität Bochum (2014)

J. V. Görler
Mesoscopic simulation of the influence of misfit dislocations on the morphology of the γ'-phase in Ni-Base superalloys
Master Thesis, Ruhr-Universität Bochum (2014)

W. Arif
Superalloy single crystal creep deformation modelling by crystal plasticity finite element method
Master Thesis, Ruhr-Universität Bochum (2014)

M. B. Addis
Lattice Boltzmann studies of non-Newtonian fluids
Master Thesis, Ruhr-Universität Bochum (2014)

T. Katiyar
Phase-field study of mechanically driven grain growth
Master Thesis, Ruhr-Universität Bochum (2014)

F. Falsafi
Thermophysical properties of Ti and Ni-Ti alloys: first-principle calculations compared to evaluated emperimental results
Master Thesis, Ruhr-Universität Bochum (2014)

M. U. Ilyas
Lagrangian dynamics simulation of cubic to tetragonal martensitic phase transformations
Master Thesis, Ruhr-Universität Bochum (2014)

L. Govinda Sharma
Effect of martensite fraction on cooling rate and grain size
Master Thesis, Ruhr-Universität Bochum (2014)

H. I. Sözen
Ab initio investigation on the energetics and kinetics of defects in Fe-Al alloys
Master Thesis, Ruhr-Universität Bochum (2014)

A. Zendegani
Modelling the morphological instability of the oxidation front in binary alloys by phase-field
Master Thesis, Ruhr-Universität Bochum (2014)

N. S. Gunda
Coarse grained lattice dynamics using compressive sensing
Master Thesis, Ruhr-Universität Bochum (2014)

Talks and Posters

14. Talks and Posters

>> Invited talks

15.01.2014
M. Kanani
Multi-scale modelling of materials: general introduction
School of Engineering's Scientific Lectures, Shiraz, Iran

31.01.2014
J. Rogal
Atomistic simulations of dynamical interface properties during phase transformations
Kolloquium für Kristallographie und technische Mineralogie, München, Germany

05.02.2014
G. Madsen
High throughput screening of thermoelectric materials
Seminar at Peter-Gründberg Institute, Jülich, Germany

17.02.2014
S. G. Fries, M. Palumbo, A. A. Breidi, J. Koßmann, T. Hammerschmidt, S. Neumeier, M. Göken
A many fold way to model the thermodynamics of Co-Al-W
TMS Annual Meeting, San Diego, USA

20.02.2014
S. V. Divinski, H. Edelhoff
Diffusion and segregation of Ag in Cu near special grain boundaries
TMS Annual Meeting, San Diego, USA

20.02.2014
S. V. Divinski, G. Reglitz, J. Fiebig, M. Wegner, M. Peterlechner, J. Leuthold, G. Wilde
Grain boundaries in severely deformed metals: effect of deformation temperature and stacking fault energy
TMS Annual Meeting, San Diego, USA

05.03.2014
G. Madsen
High throughput search for thermoelectric materials: computational stability, transport and doping properties
APS March Meeting, Denver, USA

11.03.2014
J. Rogal
Structural phase transformations in solids: atomistic insight on mechanisms and interface properties
Thomas Young Centre, London, UK

21.03.2014
G. Madsen
Data-driven materials design
45th IFF Spring School, Jülich, Germany

01.04.2014
S. V. Divinski
Grain boundaries in metals: phase and structure transitions studied by tracer diffusion
DPG-Frühjahrstagung 2014, Dresden, Germany

16.04.2014
T. Hickel
Understanding complex materials at finite temperatures by ab inito methods
Physikalisches Kolloquium der TU Chemnitz, Germany

23.04.2014
G. Madsen
The XC in DFT
ViCoM Young Researchers Meeting, Vienna, Austria
28.04.2014

D. Prokoshkina, L. Klinger, G. Wilde, E. Rabkin, S. V. Divinski
Short-circuit diffusion in recrystallizing microstructure: diffusion properties of a recrystallization front
NIST Diffusion Workshop Series, Multicomponent Diffusion Data and the Materials Genome, Gaithersburg, USA

30.04.2014
R. Darvishi Kamachali, C. Schwarze, I. Steinbach
The influence of vacancy- and particle drag on coarsening in nanocrystalline metals
MiFuN Workshop, Duisburg, Germany

07.05.2014
G. Madsen
Good vibrations: insights into the thermoelectric transport properties from Boltzmann transport theory
Arbeitsgruppenseminar at Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

08.05.2014
T. Hickel
Ab initio basierte Methoden der mechanismen-orientierten Werkstoffentwicklung
Materialwissenschaftliches Kolloquium der Salzgitter Mannesmann Forschung, Duisburg, Germany

08.05.2014
G. Madsen
Calculating the thermoelectric properties of zinc antimonides
Thermoelektrik-Kolloquium, DLR-Institut für Werkstoff-Forschung, Köln, Germany

12.05.2014
J. Frenzel
Introduction to shape memory and pseudoelasticity
SMST Conference 2014, Educational Workshop, Asilomar/Pacific Grove, USA

15.05.2014
J. Frenzel, A. Wieczorek, B. Maaß, M. O. Rahim, M. F. Wagner, C. Somsen, A. Dlouhy, E. George, G. Eggeler
On the effects of alloy composition on martensitic transformation in NiTi-based shape memory alloys
SMST Conference 2014, Asilomar/Pacific Grove, USA

17.06.2014
J. Rogal
Atomistic modelling of diffusion processes of light elements in metals
CIMTEC 2014: 6th Forum on New Materials, Montecatini Terme, Italy
23.06.2014

G. Madsen
Integrated computational materials discovery: from physical to materials properties
Special Talks and Seminars Series at Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

26.06.2014
T. Hammerschmidt, J. Koßmann, A. Bialon, M. Palumbo, S. G. Fries, R. Drautz
From high-throughput DFT calculations to thermodynamic functions
1st International Workshop on Software Solutions for ICME, Rolduc, The Netherlands

02.07.2014 - 03.07.2014
R. Janisch
Modeling and understanding interface behaviour by means of atomistic simulations
Summerschool "Interfaces" of the SFB 986 "Maßgeschneiderte Multiskalige Materialsysteme", Drochtersen-Hüll, Germany

03.07.2014
G. Wilde
Grain boundaries and triple junctions in severely deformed materials
International conference on materials by severe plastic deformation, NanoSPD, Metz, France

03.07.2014
S. V. Divinski
Microstructure - texture - grain boundary property relationship in SPD-processed metals
International conference on materials by severe plastic deformation, NanoSPD, Metz, France

04.07.2014
R. Janisch
Insights into mechanical properties of interfaces via atomistic simulations
Seminar at Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

15.07.2014
A. Hartmaier
What does nanoscale testing and modeling teach us on macroscopic material behavior?
Gordon Research Conference on Thin Films and Small Scale, Boston, USA

16.07.2014
R. Drautz
Phase stability and bond order potentials in complex phases
Compositionally Complex Alloys 2014, Munich, Germany

18.08.2014
J. Rogal
Structural phase transformations in solids: atomistic insight on mechanisms and interface properties
Energy Landscapes Symposium and Workshop, Durham, UK

18.08.2014
G. Wilde
Grain boundaries in severely deformed metallic materials
International Conference on Diffusion in Materials DIMAT 2014, Münster, Germany

26.08.2014
S. G. Fries
Co-based super alloys database, a mixed approach: experiments, first-principles and modeling
PFM2014 - 3rd International Symposium on Phase-field Method, State College, USA

02.09.2014
G. Wilde
Grain boundaries in severely deformed metals and alloys
35th Risø International Symposium on Materials Science, Risø, Denmark

04.09.2014
T. Hammerschmidt
Phase stability and elasticity from first-principles
Hero-M/ICAMS Workshop, Weeze, Germany

16.09.2014
I. Steinbach
Thermodynamic and kinetic simulation of microstructure evolution
OPTIMoM Conference, Oxford, UK

18.09.2014
V. Yardley
Orientation relationships and morphology in fcc-bct martensitic transformations: phenomenological theory and EBSD investigations
Advanced Steels: Challenges in Steel Science & Technology, Madrid, Spain

25.09.2014
I. Opahle
Shape memory alloys and caloric materials - some insights from DFT
Seminar of Materials Theory Division, Department of Physics and Astronomy, Uppsala, Sweden

01.10.2014
A. Hartmaier, K. Chockalingam, R. Hameed, X. Pang, A. M. Tahir, R. Janisch, A. Ma
Atomistically informed continuum models for plasticity and fracture of martensitic steels
24th International Workshop on Computational Mechanics of Materials, Madrid, Spain

02.10.2014
A. Monas, O. Shchyglo, S. Kim, C. Yim, D. Höche, I. Steinbach
Mg-Al alloy solidification with secondary phase precipitation
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, South Korea

02.10.2014
I. Steinbach
Why solidification? Why phase-field?
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, South Korea

02.10.2014
R. Darvishi Kamachali, S. Kim, I. Steinbach
Phase-field study of grain growth, recrystallization and texture evolution in AZ31 magnesium sheets
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, South Korea

02.10.2014
R. Drautz
Bond-order potentials: from the electronic structure to million atoms simulations
SES Annual Technical Meeting, West Lafayette, USA

06.10.2014
C. Begau, G. Sutmann
Dynamic load balancing and defect detection
CECAM Workshop - Particle-based Simulations for Hard and Soft Matter, Stuttgart, Germany

14.10.2014
S. V. Divinski
Grain boundary diffusion and segregation: radiotracer studies
Lecture Series "Diffusion properties and relaxation phenomena in high-entropy alloys" at National University of Science and Technology MISiS, Moscow, Russia

16.10.2014
S. V. Divinski
Effect of severe plastic deformation on kinetic and structure properties of grain boundaries
Lecture Series "Diffusion properties and relaxation phenomena in high-entropy alloys" at National University of Science and Technology MISiS, Moscow, Russia

03.11.2014
R. Drautz
Bond-order potentials: from the electronic structure to million atoms simulations
Workshop on Force Fields: From Atoms to Materials, Jülich, Germany

04.11.2014
T. Hammerschmidt, B. Seiser, A. C. Ladines, M. Čák, D. G. Pettifor CBE FRS, R. Drautz
Modelling topologically close-packed phases in superalloys and steels
International Workshop on Advanced Materials Science, Halong, Vietnam

04.11.2014
I. Steinbach
Phase-field model for microstructure evolution at the mesoscopic scale
Autumn school on microstructural characterization and modelling of thin-film solar cells, Werder, Germany

24.11.2014
T. Hickel
Understanding complex materials at finite temperatures by ab inito methods
Kolloquium des Instituts für Materialwissenschaft der Universität Stuttgart, Germany

01.12.2014 - 03.12.2014
I. Steinbach
Phase-field simulation of dendritic growth with melt convection
1st International VDEh-Seminar, Computational Fluid Dynamics in Metallurgy, Mönchengladbach, Germany

03.12.2014
M. Palumbo
Insight on thermophysical properties and thermodynamic modeling from DFT calculations
Université Claude Bernard Lyon 1, Villeurbanne, France

12.12.2014
S. G. Fries
A call for systematic evaluation of first-principles calculated thermodynamic quantities
Seminar at KTH Royal Institute of Technology, Stockholm, Sweden

>> Talks and posters

16.01.2014
M. Palumbo
Achievements and challenges in first-principles calculations of temperature-dependent thermophysical properties
1ère Réunion sur la Thermodynamique des Matériaux Haute Température, Thiais, France

17.02.2014
T. Wang, G. Madsen, A. Hartmaier
Reduction effect on thermal conductivity of silicon by defect structures investigated from atomistic level
TMS Annual Meeting, San Diego, USA

17.02.2014
T. Hammerschmidt, B. Seiser, M. Čák, D. G. Pettifor CBE FRS, R. Drautz
Analytic bond-order potentials for dynamical simulations
TMS Annual Meeting, San Diego, USA

17.02.2014
J. Koßmann, R. Drautz, T. Hammerschmidt
Stability of TCP phases in Co-based superalloys: comparison of ab initio results with structure maps
TMS Annual Meeting, San Diego, USA

17.02.2014
T. Hammerschmidt, B. Seiser, M. Čák, D. G. Pettifor CBE FRS, R. Drautz
Analytic bond-order potentials for dynamic simulations
TMS Annual Meeting, San Diego, USA

18.02.2014
I. Opahle
Electronic and magnetic properties of Ni_2MnGa and RT_5 alloys
TMS Annual Meeting, San Diego, USA

19.02.2014
R. Janisch, X. Pang, A. M. Tahir, A. Hartmaier
Modelling and understanding the strength of grain boundaries based on ab initio results
TMS Annual Meeting, San Diego, USA

19.02.2014
S. Schreiber, T. Hammerschmidt, R. Drautz
Analytic bond-order potentials for Fe and Fe-C
TMS Annual Meeting, San Diego, USA

25.02.2014
R. Hameed, M. Boeff, A. Ma, V. Yardley, A. Hartmaier
Micromechanical modelling of tempered martensite
Schöntal symposium on dislocation based plasticity, Schöntal, Germany

03.03.2014
C. Bera, L. Bjerg, A. Katre, G. Madsen
Thermal conductivity of nano structure materials
APS March Meeting, Denver, USA

17.03.2014
P. S. Engels, E. Borukhovich, O. Shchyglo, A. Ma, I. Steinbach, A. Hartmaier
Coupling crystal plasticity and phase-field methods
Winter School International Seminar on Process Chain Simulation and Related Topics, Karlsruhe, Germany

17.03.2014
S. Gupta, A. Ma, A. Hartmaier
Crystal plasticity phase transformation model for metastable austenitic stainless steel
Winter School International Seminar on Process Chain Simulation and Related Topics, Karlsruhe, Germany

17.03.2014
M. Kanani, R. Janisch, A. Hartmaier
Mechanical properties of interfaces in TiAl α_2/γ lamellar microstructures: atomistic study
Winter School International Seminar on Process Chain Simulation and Related Topics, Karlsruhe, Germany

17.03.2014
M. Boeff, A. Hartmaier
Application of J2- and crystal plasticity to cyclic loading conditions: accumulation of plastic strains
Winter School International Seminar on Process Chain Simulation and Related Topics, Karlsruhe, Germany

25.03.2014
S. V. Divinski
Grain boundaries in metals: phase and structure transitions studied by tracer diffusion, diffusion related phenomena
Workshop "Science at mécanique des matériaux" at Université de Rouen, France

25.03.2014
M. Stratmann, O. Shchyglo, L. Zhang, I. Steinbach
Incorporating the CALPHAD sub-lattice approach of ordering into the phase-field model with finite interface dissipation
SiMiDe Spring School, Sundern, Germany

25.03.2014
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field study of CNT Zener drag and pinning
SiMiDe Spring School, Sundern, Germany

26.03.2014
J. K. Zglinski, G. Laplanche, J. Pfetzing-Micklich, G. Eggeler
Nanoindentation of nickel-titanium shape memory alloys: investigation of recoverable strains
Nanobrücken 2014, Saarbrücken, Germany

27.03.2014 - 28.03.2014
M. Sharaf, P. Kucharczyk, N. Vajragupta, S. Münstermann, A. Hartmaier, W. Bleck
Steel endurance: from microstructure to fatigue properties
29th Aachen Stahlkolloquium, Aachen, Germany

27.03.2014
M. Sharaf
Steel endurance: a numerical solution to the fatigue problem
29th Aachen Stahlkolloquium, Aachen, Germany

31.03.2014
P. Thome, E. Payton, V. Yardley
Custom MTEX algorithms for EBSD investigations of spatially coupled crystallographic properties in plate martensite
EBSD 2014, London, UK

31.03.2014
A. C. Ladines, T. Hammerschmidt, R. Drautz
C, N and H binding energies in Fe_2Nb Laves phases
DPG Spring Meeting, Dresden, Germany

31.03.2014
T. Chakraborty, J. Rogal, R. Drautz
Atomistic modelling of phase transitions in Ti-Ta high-temperature shape memory alloys
DPG Spring Meeting, Dresden, Germany

31.03.2014
T. Hammerschmidt, S. Schreiber, B. Seiser, M. Ford, D. G. Pettifor CBE FRS, R. Drautz
Efficient implementation of analytic bond-order potentials
DPG Spring Meeting, Dresden, Germany

31.03.2014
A. C. Ladines, T. Hammerschmidt, R. Drautz
Influence of magnetism on the stability of binary transition-metal compounds
DPG Spring Meeting, Dresden, Germany

31.03.2014
A. Bialon, T. Hammerschmidt, R. Drautz
Three-dimensional structure maps for sp-d-bonded systems
DPG Spring Meeting, Dresden, Germany

31.03.2014
S. Schreiber, T. Hammerschmidt, R. Drautz
Analytic bond-order potentials for Fe and Fe-C
DPG Spring Meeting, Dresden, Germany

31.03.2014
A. Katre, R. Drautz, G. Madsen
First principles study of thermal conductivity cross-over in nanostructured zinc-chalcogenides
DPG Spring Meeting, Dresden, Germany

31.03.2014
T. Schablitzki, J. Rogal, R. Drautz
Atomistic simulation of transformations at disordered FeCr bcc-σ interfaces
DPG Spring Meeting, Dresden, Germany

01.04.2014
C. Bera, L. Bjerg, A. Katre, G. Madsen, R. Drautz
Thermal conductivity of thermoelectric nano structure materials
DPG Spring Meeting, Dresden, Germany

01.04.2014
A. N. Harjunmaa, J. Rogal, R. Drautz, R. Terrel, S. Chill, G. Henkelman
Atomistic simulations of solid-solid phase transformations in molybdenum
DPG Spring Meeting, Dresden, Germany

01.04.2014
G. Madsen
Segregation at and structure of iron grain boundaries using parameterized electronic description
DPG Spring Meeting, Dresden, Germany

02.04.2014
S. Schuwalow, J. Rogal, R. Drautz
Solute-vacancy interaction and diffusion of selected elements in Ni-based superalloys
DPG Spring Meeting, Dresden, Germany

02.04.2014
J. Koßmann, T. Hammerschmidt, S. Maisel, S. Müller, R. Drautz
Sublattice solubility of transition metals in L12 phases in Co-based superalloys
DPG Spring Meeting, Dresden, Germany

03.04.2014
X. Pang, R. Janisch
Temperature-dependent shear behaviour of different grain boundaries in aluminum: an MD study
DPG Spring Meeting, Dresden, Germany

03.04.2014
D. Sopu, X. Pang, J. Rogal, R. Janisch, R. Drautz
Comparison of transition path sampling and metadynamics for the study of solid-liquid interface properties
DPG Spring Meeting, Dresden, Germany

12.05.2014
S. Schuwalow, J. Rogal, R. Drautz
Electronic properties and diffusion behavior of refractory elements in Ni-base superalloys: a combined DFT+kMC approach
EuroSuperalloys, Giens, France

12.05.2014
A. A. Breidi, M. Palumbo, S. G. Fries
SAPIENS model platform for Co/Ni-superalloys – integration of experimental and theoretical data
EuroSuperalloys, Giens, France

13.05.2014
S. Schuwalow, J. Rogal, R. Drautz
Diffusion of vacancies and selected d-shell alloying elements in Ni: a DFT/kMC study
EuroSuperalloys, Giens, France

28.05.2014
G. Madsen
High throughput search for thermoelectric materials: computational stability, transport and doping properties
E-MRS Spring Meeting, Lille, France

29.05.2014
J. Wang, G. Madsen, R. Drautz
Structure-property correlations for grain boundaries in bcc-iron
E-MRS Spring Meeting, Lille, France

01.06.2014
B. Sundman, M. Palumbo, U. R. Kattner, S. G. Fries
New features implemented in the Open CALPHAD software project
CALPHAD XLIII, Changsha, China

03.06.2014
S. Gupta, A. Ma, A. Hartmaier
Crystal plasticity phase transformation model for metastable austenitic stainless steel
3rd International workshop on physics-based models and experimental verification, Cesme, Turkey

04.06.2014
M. Stratmann, L. Zhang, O. Shchyglo, I. Steinbach
Phase-field simulation of precipitation using the CALPHAD sublattice approach and thermodynamic databases
Calphad XLIII, Changsha, China

05.06.2014
I. Roslyakova, B. Sundman, H. Dette
Modeling of thermo-physic properties for pure elements using segmented regression methodology
Calphad XLIII, Changsha, China

11.06.2014-13.06.2014
M. Sharaf, N. Vajragupta, S. Münstermann, P. Kucharczyk, A. Hartmaier, W. Bleck
The fatigue limit of steel: a numerical solution to the short cracks problem
FDMD II - The 2nd International Symposium on Fatigue Design & Material Defects, Paris, France

24.06.2014
I. Opahle, G. Madsen, R. Drautz
Coarse grained models for large-scale atomistic simulations of spin and lattice dynamics
SPP 1599 Convention, Meißen, Germany

07.07.2014
I. Roslyakova, B. Sundman, H. Dette
Contribution to the third generation CALPHAD databases using segmented regression approach: new description for pure Cr, Al and Fe and comparison with existing models
ICAMS Advanced Discussions, Bochum, Germany

08.07.2014
S. Schuwalow, J. Rogal, R. Drautz
Solute-vacancy interaction and diffusion of selected elements in Ni-base superalloys
ICAMS Advanced Discussions, Bochum, Germany

10.07.2014
P. Thome, M. Ersanli, E. Payton, V. Yardley
In-depth EBSD investigation of spatially coupled crystallographic properties of martensite in Fe-Ni alloys
ICOMAT - International Conference on Martensitic Transformations, Bilbao, Spain

27.07.2014
I. Roslyakova, I. Steinbach, Z. Liu, U. R. Kattner
Future data mining strategies
5th Sino German Symposium, Bochum, Germany

28.07.2014
S. Schuwalow, J. Rogal, R. Drautz
Vacancy mobility and interaction with transition metal solutes in Ni
5th Sino-German Symposium, Bochum, Germany

28.07.2014
J. Koßmann, M. Palumbo, T. Hammerschmidt, R. Drautz, S. G. Fries
First-principles-based calculations of Al-base phase diagrams
5th Sino-German Symposium, Bochum, Germany

28.07.2014
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field simulation of spinodal decomposition in Al alloys
5th Sino-German Symposium, Bochum, Germany

02.08.2014
J. V. Görler
Long-term aging and coherency effects in γ/γ' forming superalloys
Symposium on Simulation of Phase Transformation and Microstructure Evolution of Materials, Changwon, South Korea

17.08.2014
T. Chakraborty, J. Rogal, R. Drautz
Stability of different competing phases in Ti-Ta high temperature shape memory alloys
Summer School on Electronic Structure Theory and Materials Design, Lyngby, Denmark

18.08.2014
J. Rogal, A. N. Harjunmaa, T. Schablitzki, R. Drautz
Structural phase transformations in solids - atomistic insight on mechanisms and interface properties
Energy Landscapes, Symposium and Workshop, Durham, UK

26.08.2014
A. Monas, O. Shchyglo, D. D. Pawlik, D. Höche, I. Steinbach
Large scale simulations of Mg-Al alloy solidification using OpenPhase
PFM 2014 – 3rd International Symposium on Phase-field Method, State College, USA

28.08.2014
P. S. Engels, E. Borukhovich, I. Steinbach, A. Hartmaier
An integrated crystal-plasticity and phase-field simulation framework
EMMC14 - European Mechanics of Materials Conference, Gothenburg, Sweden

29.08.2014
O. Shchyglo, E. Borukhovich, P. S. Engels, A. Monas, R. Darvishi Kamachali, M. Stratmann, D. Medvedev, I. Steinbach
OpenPhase - the open source phase field simulation library
PFM 2014 – 3rd International Symposium on Phase-field Method, State College, USA

04.09.2014
J. Rogal
Diffusion coefficients from atomistic simulations
Hero-M/ICAMS Workshop, Weeze, Germany

07.09.2014
M. Palumbo, S. G. Fries, A. Pasturel, D. Alfe
First-principles-based calculations of temperature-dependent thermodynamic properties of intermetallic compounds
TOFA, Brno, Czech Republic

07.09.2014
M. Palumbo, J. Koßmann, G. Cacciamani, S. G. Fries, T. Hammerschmidt
A systematic DFT-based analysis of binary phase diagrams in the Bragg-Williams approximation
TOFA, Brno, Czech Republik

13.09.2014
J. V. Görler, S. Brinckmann, O. Shchyglo, I. Steinbach
Long-term aging and coherency effects in γ/γ' forming superalloys
Modelling and simulation of superalloys, Workshop, Bochum, Germany

15.09.14
A meso-scale approach to superalloys microstructure modeling
M. K. Rajendran
Department of Scale Bridging Thermodynamic and Kinetic Simulation, Ruhr-Universität Bochum, Bochum, Germany

16.09.14
Vacancy mobility and interaction with transition metal solutes in Ni
S. Schuwalow
Department of Atomistic Modelling and Simulation, Ruhr-Universität Bochum, Bochum, Germany
17.09.14

16.09.2014
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field simulation of spinodal decomposition in Al alloys
OPTIMoM Conference, Oxford, UK

19.09.2014
J. Frenzel, M. O. Rahim, A. Wieczorek, M. Frotscher, R. Steegmüller, M. Wohlschlögel, G. Eggeler
Zum Einfluss von Karbiden und Oxiden auf die Ermüdungslebensdauer von NiTi
5. Bochumer Kolloquium für martensitische Transformation, Bochum, Germany

23.09.2014
J. K. Zglinski, G. Laplanche, J. Pfetzing-Micklich, G. Eggeler
Nanoindentation of nickel-titanium shape memory alloys: investigation of recoverable strains
Materials Science and Engineering MSE, Darmstadt, Germany

23.09.2014
O. Shchyglo, E. Borukhovich, P. S. Engels, A. Monas, I. Steinbach
OpenPhase - the open source phase field simulation library
Materials Science and Engineering MSE, Darmstadt, Germany

23.09.2014
M. Tegeler, O. Shchyglo, A. Monas, I. Steinbach, G. Sutmann
Efficient parallelization of OpenPhase for massively parallel computers
Materials Science and Engineering MSE, Darmstadt, Germany

24.09.2014
M. Kanani, R. Janisch, A. Hartmaier
Atomistic study of deformation mechanisms in TiAl-Ti_3Al lamellar microstructure
Materials Science and Engineering MSE, Darmstadt, Germany

24.09.2014
M. Stratmann, L. Zhang, O. Shchyglo, I. Steinbach
Phase-field model with Gibbs energy formulation using the sublattice formalism
Materials Science and Engineering MSE, Darmstadt, Germany

24.09.2014
M. Sharaf, S. Münstermann, N. Vajragupta, P. Kucharczyk, A. Hartmaier, W. Bleck
Structural steel endurance: towards the optimum microstructure fatigue resistance
Materials Science and Engineering MSE, Darmstadt, Germany

24.09.2014
C. Schwarze, R. Darvishi Kamachali, I. Steinbach
Phase-field study of Zener drag and pinning in carbon nanotube reinforced nano-crystalline materials
Materials Science and Engineering MSE, Darmstadt, Germany

03.10.2014
M. Sharaf, S. Münstermann, P. Kucharczyk, A. Hartmaier, W. Bleck
The optimum microstructure fatigue resistance: a micromechanical solution to an inferential statistics problem
XXIV International Workshop on Computational Micromechanics of Materials, Madrid, Spain

07.10.2014
J. Rogal, A. N. Harjunmaa, R. Drautz
Structural phase transformations in solids – atomistic insight on mechanisms and interface properties
7th International Conference on Multiscale Materials Modeling, Berkeley, USA

27.10.2014
S. Schreiber, T. Hammerschmidt, R. Drautz
Analytic bond order potentials for Fe and Fe-C: application to screw dislocations
Ab-initio description of iron and steel (ADIS): Multiple Impacts of Magnetism, Tegernsee, Germany

28.10.2014
R. Drautz
Magnetic analytic bond-order potentials: application to Fe, Mn and Fe-C
Ab-initio description of iron and steel (ADIS): Multiple Impacts of Magnetism, Tegernsee, Germany

02.12.2014
I. Opahle, G. Madsen, R. Drautz
Coarse grained models for large scale atomistic simulations of spin and lattice dynamics
SPP 1599 Focus Meeting A, Bielefeld, Germany

11.12.2014
S. Gao, M. K. Rajendran, M. Fivel, A. Ma, O. Shchyglo, A. Hartmaier, I. Steinbach
3D discrete dislocation dynamics study of plastic deformation in various Ni-base single crystal superalloy microstructures obtained by phase-field method
International Workshop on Dislocation Dynamics Simulations: Trends and Challenges, Saclay, France

Seminars and other Lectures

15. Seminars and other Lectures

>> Organisation and contribution to organisation of workshops and events

24.08.-29.08.2014
Condensed Matter 2014
Université Paris Descartes
Paris
France

26.08.-29.08.2014
PFM 2014 – 3rd International Symposium on Phase-field Method
Pennsylvania State University
State College
USA

13.09.-17.09.2014
International workshop on modelling and simulation of superalloys
Ruhr-Universität Bochum
Bochum
Germany

23.09.-25.09.2014
Materials Science and Engineering Conference
Technische Universität Darmstadt
Darmstadt
Germany

03.12.14
PolyRUB Day - Polymers for engineering applications: experiment, continuum modeling and molecular simulation
Ruhr-Universität Bochum
Bochum
Germany

08.07.- 09.07.2014
ICAMS Advanced Discussions
Ruhr-Universität Bochum
Bochum
Germany

>> RUB Seminar Materials Science and Technology (ICAMS, IfM, ZGH)

16.01.14
Stresses which affect the microstructure of Ni-base superalloys
U. Glatzel
Universität Bayreuth, Bayreuth, Germany

23.01.14
Tribocorrosion: concepts and applications
S. Mischler
École Polytechnique féderale de Lausanne, Lausanne, Switzerland

10.04.14
Mechanisms of ultra-light sliding wear
A. Fischer
Universität Duisburg-Essen, Duisburg, Germany

08.05.14
New methods for the mechanical characterization of polymers and the entropy wheel
M. Wilhelm
Karlsruher Institut für Technologie, Karlsruhe, Germany

05.06.14
Preparation and characterization of thin film energy materials: photo voltaic, photo synthesis and batteries
W. Jaegermann
Technische Universität Darmstadt, Darmstadt, Germany

03.07.14
Plasticity in hard materials – testing at small scales and high temperatures
S. Korte-Kerzel
RWTH Aachen, Aachen, Germany

10.07.14
Simultaneous evolution of microstructure and precipitation – state of the art modelling with MatCalc
E. Kozeschnik
Vienna University of Technology, Vienna, Austria

16.10.14
Modeling the static mechanical properties of magneto-sensitive elastomers
M. Grenzer
Leibniz Institut für Polymerforschung, Dresden, Germany

30.10.14
Integrated computational materials engineering – a case study on porosity from cast micropores to porous bone structures
A. Burblies
Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung, Bremen, Germany

27.11.14
Recent advances in powder metallurgical research in Sweden
A. Strondl
Swerea KIMAB AB, Kista, Sweden

>> ICAMS Seminars and other Lectures

20.01.14
CALPHAD modelling and database design
A. Watson
University of Leeds, Leeds, UK

22.01.14
Crack initiation in fatigued 316L: a 3D dislocation dynamics investigation
M. Fivel
Université Grenoble Alpes, Saint Martin d'Heres, France

19.02.14
Research at the Institute of Forming Technology and Lightweight Construction
E. Tekkaya
Technische Universität Dortmund, Dortmund, Germany

14.04.14
Design and development of fracture property measurement techniques at the small-scale and its application to intermetallics
N. J. Balila
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

16.05.14
Hydrogen in thin film systems
M. Getzlaff
Universität Düsseldorf, Düsseldorf, Germany

24.06.14
First principles-design of rhenium-based alloys for improved ductility and lower cost
M. de Jong
University of California, Berkeley, USA

03.07.14
Why to do re-assessments? The example of Co-Ta
U. R. Kattner
Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, USA

08.07.14
Data repositories for accelerated development of CALPHAD descriptions
U. R. Kattner
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08.07.14
Multiplicity of grain boundary structures and its consequences
V. Vitek, J. Han
University of Pennsylvania, Philadelphia, USA

09.07.14
Calculation of stacking fault and anti-phase boundary energies in fcc alloys using only a thermodynamic data base
P. Miodownik
Surrey Technology Centre, Sente Software Ltd., ThermoTech Ltd., Guildford, UK

09.07.14
CALPHAD modelling applied to the simulation of metallic materials in general and to cobalt-based superalloys in particular
G. Cacciamani
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09.07.14
Importance of screening of bond integrals in BOPs for transition metals
V. Vitek, Y. Lin, M. Mrovec
University of Pennsylvania, Philadelphia, USA and Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany

12.08.14
A joint APT/TEM approach to study co-deformation of amorphous/nanocrystalline nanolaminates
W. Guo
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17.09.14
Materials by design: from the nanoscience to the macromechanics of modern steel alloys
T. M. Hatem, P. Shanthraj
British University in Egypt, Cairo, Egypt and Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

26.09.14
Entropy
Z. Liu
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07.10.14
Nanostructure design via non-conventional phase transformation pathways in multi-phase alloys
Y. Wang
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29.10.14
Capturing the complex physics behind universal grain size distributions in thin metallic films
A. Voigt
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Collaborations, Guests and Visitors

16. Collaborations, Guests and Visitors

>> Guests and visiting scientists

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Teaching and Lectures

17. Teaching and Lectures

>> Lecture courses summer term 2014

A. Hartmaier, I. Steinbach
Microstructure and mechanical properties

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

S. G. Fries
The CALPHAD method

G. Madsen, J. Neugebauer, I. Opahle
Application and implementation of electronic structure methods

T. Hammerschmidt
Quantum mechanics in materials science

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

>> Lecture courses winter term 2014/15

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

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

V. Yardley
Elements of microstructure

E. George
Materials processing

A. Hartmaier, I. Steinbach
Continuum methods in materials science

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

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

A. Ma, G. Madsen
Programming concepts in materials science

R. Drautz
Atomistic simulation methods

J. Rogal
Advanced atomistic simulation methods

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

T. Hickel
Introduction to quantum mechanics

A. Hartmaier
Numerical simulation of fracture of materials

F. Varnik, R. Spatschek
Statistical physics and thermodynamics

I. Steinbach
Solidification processing

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

>> Other courses

J. Neugebauer, R. Drautz, I. Steinbach, A. Hartmaier
Multiscale modelling in materials science basic course

S. Sampath, J. Rogal, S. G. Fries, F. Varnik, M. Čák, T. Hammerschmidt, A. Ma, K. Chockalingam, R. Spatschek
Multiscale modelling in materials science advanced course

R. Drautz, J. Yates
Introduction to modelling in materials science
University of Oxford, Oxford, UK

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