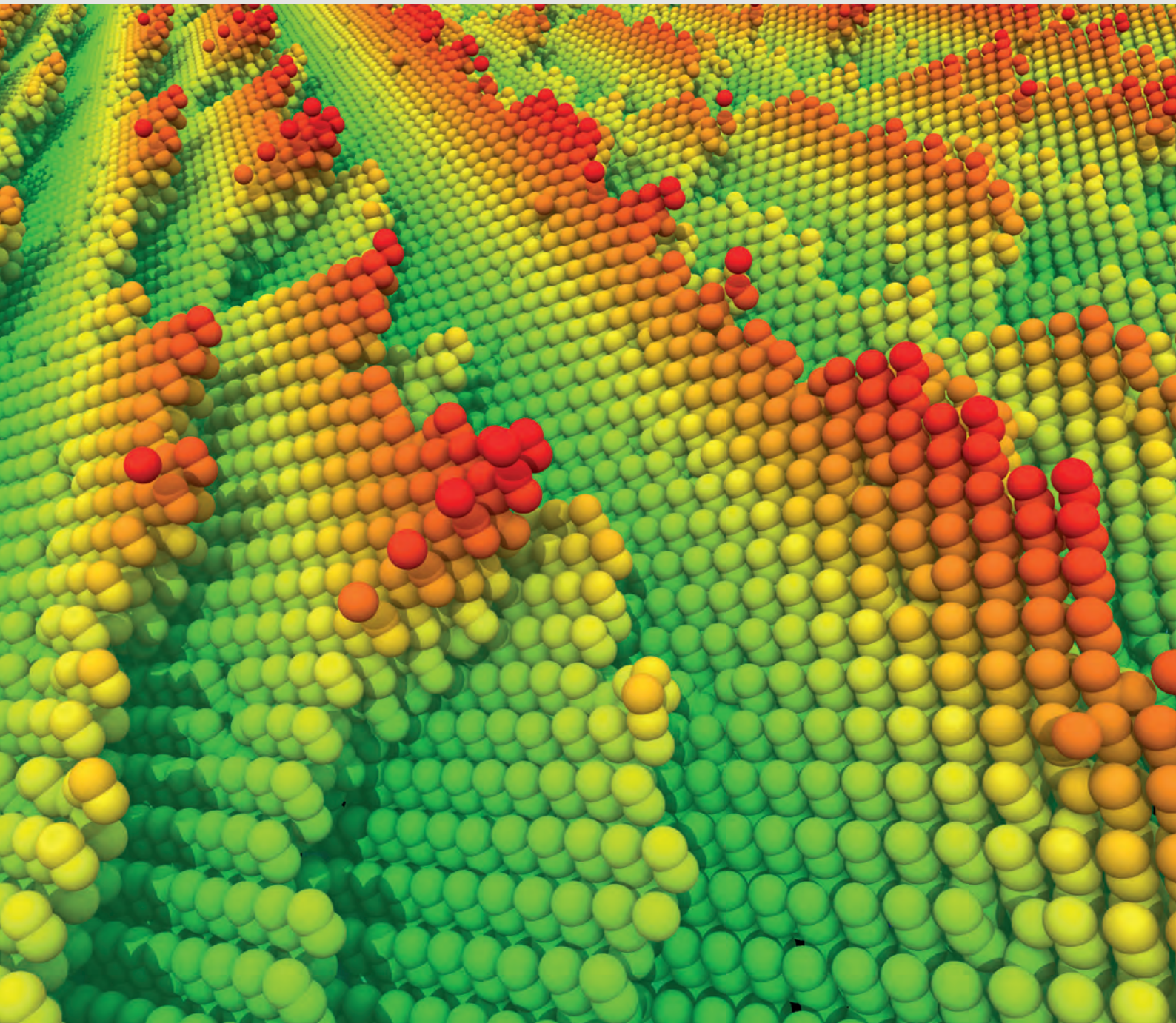
MAX-PLANCK-GESELLSCHAFT

Scientific Report 2013 - 2015

Max-Planck-Institut
für Eisenforschung GmbH



Max-Planck-Institut für Eisenforschung GmbH

Scientific Report 2013 - 2015

November 2015
Max-Planck-Institut für Eisenforschung GmbH
Max-Planck-Str. 1 · 40237 Düsseldorf
Germany

Front cover

The figure shows a snapshot of a moving grain boundary obtained by large-scale molecular dynamics simulations in the Department of Computational Materials Design. In contrast to previous studies, mesoscale features such as the migration via steps and kink sites are accurately included. The figure shows only the lower grain while atoms of the upper grain have been rendered invisible for clarity. The color indicates the height profile of the atoms. The direction normal to the grain boundary has been stretched to emphasize the step structure.

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Imprint

Published by
Max-Planck-Institut für Eisenforschung GmbH
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Homepage: http://www.mpie.de

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Printed by
Bonifatius GmbH
Druck-Buch-Verlag
Paderborn, Germany

PREFACE

This report documents the scientific activities and achievements of researchers at the Max-Planck-Institut für Eisenforschung GmbH (MPIE) between 2013 and 2015. Moreover, we present some long-term methodological developments in the fields of computational materials science, advanced microstructure characterization, electrochemistry and synthesis.

The mission of the MPIE lies in understanding and designing complex nanostructured materials under real environmental conditions down to the atomic and electronic scales. More specific, the Institute conducts basic research on structural and functional materials, specifically steels and related alloys, considering their complex chemical-physical synthesis, characterization and properties, as well as their use in systemic components and under harsh environmental conditions.

Projects are conducted highly interdisciplinary, in an atmosphere of permanent mutual stimulation among experimentalists and theoreticians as well as among the different departments. The methodological interplay reaches from macroscopic and combinatorial synthesis up to thermomechanical processing of novel alloy classes through the observation of individual atoms by high resolution electron microscopy and atomic probe tomography, closely flanked by corresponding through-process and atomistic simulations.

The MPIE laboratories and simulation groups cover the entire synthesis, processing, microstructure and property chain, i.e. the materials development and understanding include and control the entire history of every specimen. Due to our interdisciplinary research approach we defined a number of core topical areas:

- Development of new structural materials
- Analysis of microstructure-related material properties
- Analysis and enhancement of the stability of surfaces and interfaces
- Development of scale-bridging simulation of materials
- Enhancement of energy materials

Through its focus on advanced complex materials the MPIE occupies a key role in enabling progress in a number of fields such as

- Mobility (e.g., ductile magnesium sheet alloys, high strength steels and soft magnets for light weight hybrid vehicles)
- Energy (e.g., hydrogen-tolerant structural alloys, efficiency of thermal power conversion through better high temperature alloys, semiconducting materials for photovoltaics and photo-electrochemistry, fuel cell components)
- Infrastructure (e.g., steels for large infrastructures such as wind turbines and chemical plants)
- Health (e.g., development of elastically soft titanium hip implants)
- Safety (e.g., nanostructured bainitic steels for gas pipelines).

We conduct projects with strong rooting in knowledge-oriented and pre-competitive basic research on the one hand and include aspects associated with the application and commercial relevance of the materials, processes and methods on the other hand. With its system-oriented research agenda and its institutional co-sponsoring by industry, the Institute constitutes a unique example of public-private partnership both, for the Max Planck Society and for the European industry.

Strengthening of the Institute's scientific profile is achieved by strategic collaborations with several academic partners, namely, R. Kirchheim (materials physics and atom scale characterization; University of Göttingen) who is external scientific member of the Max Planck Society, J. Schneider (combinatorial and thin film materials design; RWTH Aachen University) who is Fellow of the Max Planck Society, and G. Eggeler (high temperature alloys and energy-related materials; Ruhr-Universität Bochum) who is external group leader at the MPIE. With these colleagues a number of very close joint projects are pursued (e.g. exploring the limits of strength in Fe−C systems; hydrogen-propelled materials and systems; defectant theory; creep of superalloys; self-reporting and damage tolerant materials; atomic scale analysis of interfaces in superalloys and hard coatings).

The Institute hosts currently about 300 people, the majority being scientists. As 180 employees are funded by the basic budget provided by the shareholders of the Institute, around 120 additional scientists work at the MPIE supported by extramural sources such as the ERC, DFG, RFCS, AvH, DAAD, BMBF, BMWi and CRC to name but a few essential funding agencies.

An increasing number of co-operations with strategically selected industrial partners has provided further extramural momentum to the dynamic growth of the MPIE during the past three years. Besides the well established links to the steel industry and related companies in the domains of alloy design (bulk and surface), advanced characterization, surface functionalization, and computational materials science, new industrial co-operations were established in a number of novel fields: These new project directions are particularly valuable for the Institute's further development from a materials-oriented laboratory towards a system-driven institute developing complex materials in a holistic approach. This approach carries complicated engineering systems and environmental conditions into advanced materials science and manufacturing processes. New areas of growth including strong interactions with industry are in the fields of steels and related materials for automotive hybrid- and electro-mobility, energy conversion and storage, renewable energy, health, hydrogen-based industries, and computational materials science. This contribution of third-party funds and its balance between fundamental and applied science places the MPIE into a singular position within the Max Planck Society.

Further scientific momentum is currently fueled by the requirement for a better understanding of the often complex interactions between electrochemistry and microstructure. Modern materials are both, enabled and limited by the presence of interfaces and surfaces and their reactivity with the environment. This stimulates new experimental and theoretical projects at the MPIE in the fields of atomic scale and in-situ reaction analysis at interfaces regarding electrochemistry, transport, reactions and damage; hydrogen effects; combinatorial surface-electrochemistry; in-situ and multi-probing of interfaces; corrosion protection; interface cohesion and solid-liquid interfaces.

MPIE researchers have achieved several scientific breakthroughs in the past years such as the development of 7 GPa strong pearlitic steels, observation of mechanically induced martensite formation by severe plastic deformation, joint structural and chemical characterization of segregation in nanocrystalline steels and semiconductors at the atomic scale, development of long-term reliable corrosion sensitive self-healing coating systems, derivation of a scaling strategy predicting large-scale properties such as adhesion or cell-cell interactions on the basis of single-molecule measurements, design criteria to control the fracture toughness in metallic glasses, the discovery of linear confined structural and chemical states (complexions) at dislocations, understanding the complex interplay between vibronic and magnetic degrees of freedom in steels, the discovery of novel 2D interfacial phases in complex oxides, linking transport properties in semiconducting phases to growth conditions and defects and understanding degradation mechanisms in energy generating devices. These recent highlights were enabled by a number of long-term methodological projects which led to a variety of novel experimental and simulation tools. Examples are the combinatorial corrosion and catalysis probing cell, the scanning Kelvin probe, correlative atom probe tomography (TEM analysis conducted on the same specimens), the simulation toolbox DAMASK, the wet chemical cell for in-situ reaction analysis in TEM, high precision *ab initio* simulation methods, development of automated computational tools for high-throughput calculations, and development of site specific mechanical testing strategies under environmental conditions.

This report is structured into four parts:

- Part I presents the organization of the Institute including a short section on recent scientific developments, new scientific groups, new scientific laboratories, long-term oriented method development and large network activities.
- Parts II and III cover the research activities of the Institute. Part II provides a description of the scientific activities in the departments and Part III contains selected short papers which summarize major recent scientific achievements in the topical areas of common interest of the MPIE.
- Part IV summarizes some statistically relevant information about the Institute.

The Directors of the MPIE

Düsseldorf, November 2015

CONTENTS

PART I.

THE INSTITUTE

Management of the Institute

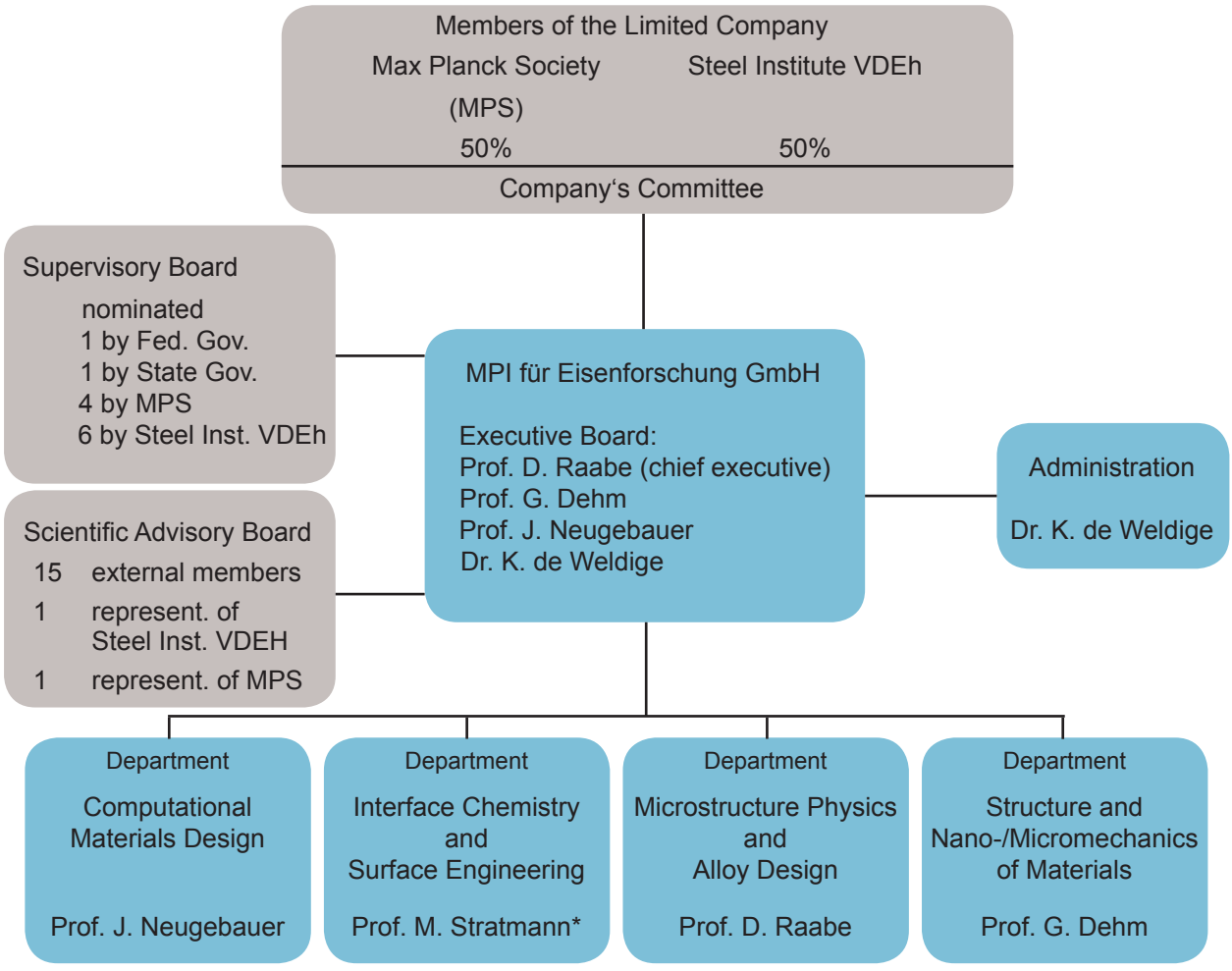
The Max-Planck-Institut für Eisenforschung GmbH (MPIE) is a joint venture between the Max Planck Society and the Steel Institute VDEh. As the Institute's budget is supplied indirectly through industry, this Institute is unique within the Max Planck Society.

The Institute was founded in 1917 by the Verein Deutscher Eisenhüttenleute (VDEh) and incorporated into the Kaiser-Wilhelm-Gesellschaft, the predecessor of the Max Planck Society. The MPIE was first located in Aachen and was associated with the Technical University of Aachen. Later, in 1934/35, the Institute moved to its present location on a site donated by the city of Düsseldorf.

In 1946, the Institute's heavily damaged buildings were reconstructed, work resumed and the MPIE was integrated into the newly formed Max Planck Society in 1948. The Institute rapidly expanded and new laboratory buildings were built in the early 1960s. Following the appointment of H.J. Engell as director in 1971, a complete reorganization of the Institute was carried out. Since then it has operated on the legal basis of a limited liability company (GmbH) and its budget is covered by the Steel Institute VDEh and the Max Planck Society.

Until 2002, the Institute was headed by a chief executive director (1971-1990: Prof. Engell, 1990-2002: Prof. Neumann) and an associated administrative director. Since June 2002, all scientific members and the administrative director of the Institute form an executive board of directors. The position of a managing director is filled, in rotation, by one of the board members. A board, which supervises the MPIE's activities, consists of representatives from the federal government, the state of North Rhine-Westphalia, the Max Planck Society and the Steel Institute VDEh. A Scientific Advisory Board comprised of prominent scientists assists the Institute in balancing fundamental research and technological relevance.

MAX-PLANCK-INSTITUT FÜR EISENFORSCHUNG GMBH
Management and Organization (Nov. 2015)



* Prof. M. Stratmann is on leave. Temporary head of the department is Prof. J. Neugebauer.

Scientific Organization

The MPIE conducts basic research on metallic alloys and related materials. It pursues an approach where material systems are studied under consideration of their highly complex underlying nanostructures on the one hand and their exposure to extreme environmental conditions on the other hand.

The Institute is divided into four departments:

- Computational Materials Design (Prof. J. Neugebauer): description of materials properties and processing based on *ab initio* (parameter free) multiscale simulation techniques
- Interface Chemistry and Surface Engineering (Prof. M. Stratmann (on leave); temporary: Prof. J. Neugebauer): aspects of environmentally accelerated degradation of surfaces and interfaces such as corrosion and deadhesion and the engineering of new and stable surfaces and interfaces
- Microstructure Physics and Alloy Design (Prof. D. Raabe): alloy design and mathematical modelling of microstructures and properties during processing and their experimental investigation using microscopy, atom probe tomography, and diffraction methods
- Structure and Nano-/Micromechanics of Materials (Prof. G. Dehm): mechanical response of materials focusing on small length scales by applying nano-/micromechanical approaches combined with advanced microstructure characterization techniques

Each department is subdivided into research groups which are typically managed by group heads. The figure on page 12 shows the organization of the groups within the departments. Each research group has its own specific focus and research activities. Part II of this report contains the summaries of the scientific concepts of the departments and brief descriptions of the research done in the different groups.

In addition to departmental research, certain research activities are of common interest within the Institute. These central research areas are highly interdisciplinary and combine the experimental and theoretical expertise available in all departments. In concerted activities, scientific and technological breakthroughs in highly competitive research areas are achieved. Selected scientific highlights including such interdepartmental research activities are described in Part III which is divided into the five topics

- Development of new structural materials
- Analysis of microstructure-related materials properties
- Analysis and enhancement of the stability of surfaces and interfaces
- Development of scale-bridging simulation of materials
- Enhancement of energy materials

For each of these five central research areas, several short papers on selected scientific topics are provided in Part III giving an overview of the results obtained during the last three years.

In summary, the research within the MPIE is organized vertically in highly specialized departments and research groups and horizontally in interdepartmental research activities. We believe that this form of organization encourages a high level of individual scientific work within the departmental framework of research groups as well as the development of new materials with complex properties combining e.g. high mechanical strength with high surface functionality. In a typical university setting, research activities such as metallurgy or surface science are carried out in different university departments. In contrast, these research activities are linked through the Institute's research structure leading to a more efficient use of the scientific equipment, a homogeneous research profile and an intense interdepartmental cooperation.

Service groups provide the scientific departments with valuable expertise. These services include the production, processing and testing of materials, chemical analysis of metallic substrates, metallography, a mechanical workshop equipped for the handling of unusually hard and brittle materials, facilities to build scientific equipment, an electronic workshop, a library, a computer network centre and a research coordination office.

Scientific Scopes of the Departments

Department **Computational Materials Design** Prof. J. Neugebauer	Department **Interface Chemistry and Surface Engineering** Prof. M. Stratmann*	Department **Microstructure Physics and Alloy Design** Prof. D. Raabe	Department **Structure and Nano-/ Micromechanics of Materials** Prof. G. Dehm
Ab Initio Calculation of Thermodynamic and Kinetic Data	Electrochemical Surface Science	Alloy Design and Synthesis	Micro-/Nanomechanics and -tribology of Materials and Interfaces
Theoretical Studies on Microstructure Properties and Dynamics	Catalysis and Corrosion	Micromechanics	In situ Methods Interlinking Mechanics and Microstructure
Computer Aided Alloy Design	Adhesion and Functional Coatings, Surfaces and Interfaces	Correlative Atom Probe Tomography	Advanced Transmission Electron Microscopy
Multiscale Modelling	Fundamental Research on Surface and Coating Related Process Technology	Segregation Engineering and Interface Manipulation	Thin Films, Nanostructured Materials and Intermetallics

* Prof. M. Stratmann is on leave. Temporary head of the department is Prof. J. Neugebauer.

Interdepartmental Research Activities

Department **Computational Materials Design** Prof. J. Neugebauer	Department **Interface Chemistry and Surface Engineering** Prof. M. Stratmann*	Department **Microstructure Physics and Alloy Design** Prof. D. Raabe	Department **Structure and Nano-/ Micromechanics of Materials** Prof. G. Dehm
Development of new structural materials			
Analysis of microstructure-related materials properties			
Analysis and enhancement of the stability of surfaces and interfaces			
Development of scale-bridging simulation of materials			
Enhancement of energy materials			

* Prof. M. Stratmann is on leave. Temporary head of the department is Prof. J. Neugebauer.

Scientific Groups and Departments (2015)

Computational Materials Design
Prof. J. Neugebauer

- Ab Initio Thermodynamics — Dr. M. Friak (until Sep. 2013)
- Adaptive Structural Materials — Dr. B. Grabowski
- Computational Phase Studies — Dr. T. Hickel
- Computer Centre — Dr. C. Freysoldt
- Defect Chemistry and Spectroscopy — Dr. C. Freysoldt
- Electrochemistry and Corrosion — Dr. M. Todorova (since Oct. 2015)
- Mesoscale Simulation — Dr. R. Spatschek (until Oct. 2015)
- ERC Starting Grant TIME BRIDGE — Dr. B. Grabowski (since Jul. 2015)

Interface Chemistry and Surface Engineering
Prof. M. Stratmann*

- Atomistic Modelling — Dr. S. Wippermann (since Feb. 2013)
- Christian Doppler Lab. for Diffusion and Segregation Mechanisms — Dr. M. Rohwerder (until Dec. 2014)
- Corrosion — Dr. M. Rohwerder
- Electrocatalysis — Dr. K. J. J. Mayrhofer
- Interaction Forces and Functional Materials — Dr. M. Valtiner
- Interface Spectroscopy — Dr. A. Erbe
- Interface Structures and High-Temperature Materials — Dr. F. Renner (until Jun. 2013)

Microstructure Physics and Alloy Design
Prof. D. Raabe

- Adaptive Structural Materials — Dr. C. Tasan
- Alloy Design and Thermomechanical Processing — Dr. D. Ponge
- Alloys for Additive Manufacturing — Dr. E. Jägle (since Apr. 2015)
- Atom Probe Tomography — Dr. P. Choi
- Biological Composites — Dr. H. Fabritius
- Combinatorial Metallurgy and Processing — Dr. H. Springer
- Interface Design of Solar Cells — Dr. O. Cojocaru-Mirédin (until Sep. 2015)
- Microscopy and Diffraction — Dr. S. Zaefferer
- Theory and Simulation — Dr. F. Roters
- Coop. with RWTH Aachen University Interface Design in Solar Cells — Dr. O. Cojocaru-Mirédin (since Sep. 2015)

Structure and Nano-/ Micromechanics of Materials
Prof. G. Dehm

- Advanced Microstructure Characterization — Dr. C. Liebscher (since Apr. 2015)
- Intermetallic Materials — Dr. M. Palm, Dr. F. Stein
- Nano-/ Micro-mechanics of Materials — Dr. C. Kirchlechner (since Mar. 2013)
- Nanotribology — Dr. S. Brinckmann (since Dec. 2014)
- Synthesis of Nanostructured Materials — N.N.
- Max Planck Research Group High Temperature Materials — Prof. G. Eggeler (since Jan. 2015)

Independent Max Planck Research Groups

- Nanoanalytics and Interfaces — Prof. C. Scheu (since Apr. 2014)

External Members and Fellows

- External Scientific Members — Prof. M. Hillert, Prof. R. Kirchheim
- Max Planck Fellow High Temperature Materials — Prof. G. Eggeler (until Dec. 2014)
- Max Planck Fellow Self-Reporting Materials — Prof. J. Schneider (since Oct. 2015)

* Prof. M. Stratmann is on leave. Temporary head of the department is Prof. J. Neugebauer.

Scientific Service Groups

- Processing — Dr. H. Springer
- Metallography — Dr. S. Zaefferer
- Materials Testing — Dr. D. Ponge
- Research Coordination Office — Dr. K. Hübel

Recent Developments

From 2012 to 2015 several major structural, scientific and administrative developments were made to further strengthen the Institute's scientific profile

The recently appointed director and executive G. Dehm started his department focusing on "Structure and Nano-/ Micromechanics of Materials". The department was opened in October 2012 and the major construction efforts, devoted particularly to hosting many of the new advanced electron microscopy facilities, will be essentially finished by mid 2016. The department works on nano- and micromechanics – mainly performed *in situ* using electron microscopy and x-ray diffraction, advanced electron microscopy characterization, nanotribology, synthesis of nano-structured and high-temperature intermetallic materials.

Also a new independent research group on "Nanoanalytics and Interfaces" has been opened by C. Scheu who joined the MPIE in April 2014. The main research activities include the atomic and electronic structure investigations of defects and interfaces in materials used for renewable energy applications. The group has initiated first collaborations with the groups of *in-situ* nano-/micromechanics and advanced electron microscopy in the department of G. Dehm, atom probe tomography and alloy design in the department of D. Raabe, electrochemical studies in the department of M. Stratmann, and plans to correlate experimentally determined bonding characteristics (via EELS) with those calculated in the department of J. Neugebauer.

The new team members complement the activities of the existing departments on "Microstructure Physics and Alloy Design" (D. Raabe), "Interface Chemistry and Surface Engineering" (M. Stratmann (on leave), temporary heads: M. Rohwerder & J. Neugebauer), and "Computational Materials Design" (J. Neugebauer). Together, the four departments cover a broad range of expertise and tools for designing, synthesizing, and analyzing complex structural materials and associated processes under harsh and reactive environmental conditions. More specific, strong intramural collaborations with the new department, exploiting particularly its electron optical and *in-situ* experimental expertise, have been established in the fields of deformation-driven phase transformations, development of ductile and tough metallic glasses, hydrogen embrittlement, strengthening mechanisms in metallic nanolaminate composites, nanostructured thermoelectric materials, chemical decomposition in martensitic alloys, density reduced high strength steels, correlative atom probe and transmission electron microscopy and complexions to name but a few of the latest projects jointly pursued. A series of inter-departmental workshops has been established to foster collaborations including also young team members and to identify new promising joint research topics of high scientific risk, gain and synergy.

In the period reviewed (end of 2012 - 2015) several new research groups have been initiated, namely, the group on "Nanotribology" by S. Brinckmann, the BMBF-funded group on "Interface Design in Solar Cells " by O. Cojocaru-Mirédin, a newly awarded ERC Starting Grant group by B. Grabowski on time-scale bridging potentials for realistic molecular dynamics simulations, a group funded by the joint Max-Planck-Fraunhofer initiative on "Alloys for Additive Manufacturing" by E. Jägle, the group for "Nano-/Micromechanics of Materials" by C. Kirchlechner, the group for "Advanced Microstructure Characterization" by C. Liebscher, and the "Atomistic Modelling" group as well as the BMBF NanoMatFutur research group „Semiconducting nanocomposites with tailored electronic and optical properties for solar energy conversion" by S. Wippermann.

A number of large-scaled and networking projects were initiated or prolonged during the last years. Examples are the European research network on „Mechanics of Nano-Objects" (MECANO) which is concerned with the mechanical properties of materials in small dimensions or the collaboration with the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) at the Ruhr-Universität Bochum. ICAMS focuses on the development and application of a new generation of simulation tools for multi-scale materials modelling.

Other initiatives include the ERC Advanced Grant funded joint group on "Adaptive Structural Materials" which jointly develops novel experimental and theoretical tools and methodologies, employing them to understand micro-mechanisms governing macro-properties and design property-optimized novel structural alloys.

The Institute pursues also several large joint initiatives with its neighbour universities RWTH Aachen University (SFB 761: Steel *ab-initio*, 3rd funding period granted by DFG; newly founded Max Planck Fellow Group on "Self-Reporting Materials" by J. Schneider) and Ruhr-Universität

Bochum (SFB/TR 103: Next Generation Single Crystalline Superalloys, 2nd funding period granted by DFG; International Max Planck Research School (IMPRS SurMat) which is managed by E. Gattermann and A. Erbe; Center for Electrochemical Sciences; external research group of the MPIE on "High Temperature Materials" by G. Eggeler). The IMPRS SurMat has been recently successfully evaluated and prolonged, extending the number of members to now also including colleagues from the University Essen-Duisburg.

Recently several group leaders of MPIE received professorship offers from prestigious universities such as from Ohio State University, University Bern, Erlangen University, RWTH Aachen University, Massachusetts Institute of Technology MIT and the Korea Institute of Science and Technology KIST.

MPIE members are also involved in several science community und service activities such as serving as vice-president and president of the Max Planck Society (M. Stratmann), as member of the reviewer panel (Fachkollegiat) of the German Research Foundation DFG (J. Neugebauer) and as member of the German Council of Science and Humanities (Wissenschaftsrat) and the Joint Strategy Commission (Strategiekommission) for the German Excellence Initiative (D. Raabe).

Several highly visible awards were won by MPIE members in the past years (end 2012 - 2015), among them an ERC Starting Grant, 4 Alexander von Humboldt Awards for Senior Professors, the Otto-Hahn Award, the NRW Innovation Award, the DECHEMA-Award and 2 BMBF Junior Research Group Awards to name but a few important recognitions.

In order to stay connected to graduates and former scientists of the Institute and to benefit from their experience MPIE established a corresponding alumni network.

A new website has been launched in spring 2015 presenting the Institute's research and achievements to different target groups ranging from scientists over students, journalists, politicians, industry representatives and school students to the wider public community. Furthermore a new series of lectures named "KopfSalat" has been started in autumn 2014 to increase the visibility of the Institute within the region. In this series high ranking scientists present their work to a broad regional public audience.

Another important transition currently affects the Institute's future institutional core funding and legal status: The MPIE is one of the longest existing Max Planck institutes since its establishment in 1917 as Kaiser-Wilhelm-Institut für Eisenforschung. In 1971 it was rendered into a company with GmbH legal form and basic budget sharing between the Max Planck Society and the German Iron and Steel Institute VDEh of 50% each. Effective as of 2016 it is intended that the institutional VDEh contribution will be stepwise reduced over a period of three years to arrive at an overall smaller permanent budget fraction. The corresponding negotiations on alternative funding and temporary cost reduction options are currently ongoing. This shift in the institutional and legal setting will be used by MPIE to sharpen and shape its scientific focus along its mission of understanding and designing complex nanostructured materials under real environmental conditions down to the atomic scale.

Independent Research Groups

Independent Max Planck Research Group on Nanoanalytics and Interfaces

Group Head: C. Scheu

Research Mission and Scientific Concepts

The independent research group "Nanoanalytics and Interfaces (NG)" (Fig. 1) was established in April 2014 and is headed by Christina Scheu who holds on the same time a full professorship at the RWTH Aachen. The main research field of the NG is the in-depth characterization of novel nanostructured materials and interfaces via electron microscopy techniques. State-of-the-art transmission electron microscopy (TEM) is employed to obtain insight into the atomic arrangement, chemical composition and bonding behaviour down to the atomic scale. The results are used to establish e.g. growth models for nanostructures and structure-properties relationships. In addition, strategies are developed to improve the properties and stability of the materials of interest. The investigated materials systems are ranging from oxides, nitrides, carbides to polymers and composites with applications in photovoltaics, fuel cells and electrochemical cells. Furthermore, thin films used for metal contacts and protective layers are studied. In part, the nanostructures and thin films are grown in our group via wet chemical synthesis or physical vapour deposition routes. In addition, we are in close cooperation with project partners developing novel materials and several of our projects are funded by third parties such as the DFG including a partial project within the SFB 761/3 "Stahl *ab initio*" (see p. 52).

Fig. 1: *The NG group at the IAMNano workshop in Hamburg (summer 2015).*

To elucidate the relationship between structure, synthesis and properties of nanostructures, we use various TEM techniques. High-resolution TEM (HRTEM) and high-angle annular dark-field (HAADF) scanning TEM (STEM) are applied to obtain information on the local arrangement of atoms and to study defects with a resolution down to the atomic scale [1, 2]. The three-dimensional morphology of nanostructures is investigated by bright-field and dark-field imaging as well as electron tomography (the latter in close cooperation with international partners [3, 4]). The chemical composition of novel materials [5, 6], individual nanostructures [2, 7, 8] and interfaces [9, 10] are analyzed by energy-dispersive X-ray spectroscopy (EDX) and electron energy-loss spectroscopy (EELS). The EELS measurements enable a localized investigation of the electronic structure and optical properties (e.g. band gap [2, 11, 12]). The bonding behaviour and oxidation state of various nanostructures is determined by analyzing the electron energy-loss near-edge structure (ELNES) of individual, element-specific edges [6, 7]. For a detailed interpretation of EELS data, *ab-initio* calculations [6, 11] or a comparison with well-defined standard materials [7] are employed. *In-situ* TEM heating experiments are currently conducted to investigate phase transformations and structural changes on an atomic scale, similar as in an early work where we discovered the *in-situ* growth of alumina nanowires [13].

The environmental pollution and the climate change on the one hand and the increasing demand of energy supply together with decreasing gas and coal resources on the other hand have intensified the research on alternative, renewable energy sources. New concepts are developed for producing and storing energy as well as fuel - like hydrogen - in an environmentally friendly way and ideally at low costs. Besides novel materials and material combinations, the morphology plays a key role. Nanostructured materials offer the advantage of a large surface area/interface area to volume ratio. This leads to more efficient light harvesting devices, which are used to convert solar energy in either chemical (water-splitting) or electric energy (solar cells). Furthermore, these nanostructures can be often synthesized in an environmentally friendly way using fast and simple synthesis strategies. The NG group has several research activities in the field of nanostructured materials for renewable energy sources as outlined in the following.

Nanostructured Materials for Photovoltaics and Photoelectrochemistry

Nanostructured, non-silicon based thin-film photovoltaic devices are potential candidates for low-cost electricity generation. In one of our research projects we synthesize $CuInS_2$ thin films and nanostructures via a solvothermal route developed earlier [14,15]. With this approach crystalline solid materials can be grown at low temperatures and in the case of $CuInS_2$ in the Chalcopyrite modification at 150 – 160 °C.Nanostructured $CuInS_2$ thin films (Fig. 2) show a strong absorption behaviour over the whole visible light spectrum, possess a direct band gap of about 1.5 eV like the bulk phase and can act as both electron or hole conductor depending on the chemical composition.and we will . The chemical composition will be analysed in more detail by EELS,EDX and atom probe investigations together with the department Microstructure Physics and Alloy Design (MA). In addition, we plan to perform electrochemical tests with the department of Interface Chemistry and Surface Engineering (GO), since $CuInS_2$ is reported to work as a photo-catalyst for light-induced splitting of water to produce hydrogen fuel, which is a central research topic of the NG (see also below).

Another research example is based on regular arrays of n-type large band gap semiconducting metal-oxide nanowires (e.g. TiO_2). These networks can be used as electrode materials in e.g. water-splitting devices or excitonic solar cells like dye-sensitized or hybrid solar cells. In the case of hybrid solar cells, the nanowire network is filled with an organic p-type semiconductor (e.g. poly(3-hexylthiophene) (P3HT)) which acts as absorber as well as a hole conductor. Due to the large interface, an efficient charge separation and thus a high efficiency is expected. However, the nanostructured photovoltaic devices lack behind the expectations. The factors limiting the performance were evaluated together with Prof. Lukas Schmidt-Mende from the University of Konstanz in project funded by the German Research Foundation (DFG). We have explored the atomic arrangement, crystal modification, band gap, and chemistry of hydrothermally grown nanowires on the atomic scale using various TEM techniques. The obtained information was correlated to the synthesis conditions and based on these results a growth model was developed which allows to explain the observed defect structures [1]. The TiO_2 nanowires crystallize in the rutile modification and exhibit facetted morphology with the {110} surface dominating. The growth is parallel to the <001> direction with a truncated growth front formed by {111} and {001} facets. The nanowires have a single crystalline bottom, but with ongoing crystal growth planar defects such as stacking faults occur, which form the starting point of a defect cascade causing

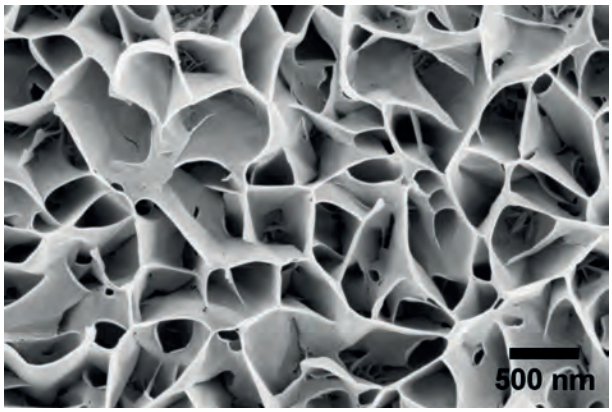


Fig. 2: *SEM image of a nanostructured $CuInS_2$ thin film synthesized by a solvothermal method in a teflon-lined stainless steel autoclave at low temperatures. The synthesis was done following a protocol published in [14,15].*

a finger-like structuring of the nanowire top (Fig. 3). This is most likely caused by steric hindrance and electrostatic repulsion at the {001} facets [1]. The occurring free surfaces as well as the stacking faults within the interior of the nanowire hinder an efficient electron transport and thus are responsible for the low efficiency of these solar cells [1, 16]. Ex-situ heating experiments performed at elevated temperatures revealed that the fingers at the nanowire top and the planar defects can be removed, but voids are formed within the nanowire interior. However, when applied in nanostructured solar cells, these voids have comparable little effect on the transport properties compared to the fingers [16]. A pronounced improvement of the cells was also achieved by creating nanowires with a highly conductive core via Sn^{4+} doping and a TiO_2 anatase shell which leads to a reduced charge carrier recombination [17]. Inspired by the promising results, we plan to do *in-situ* TEM heating experiments to uncover the structural changes occurring during the thermal treatment. In addition, a detailed study of the void

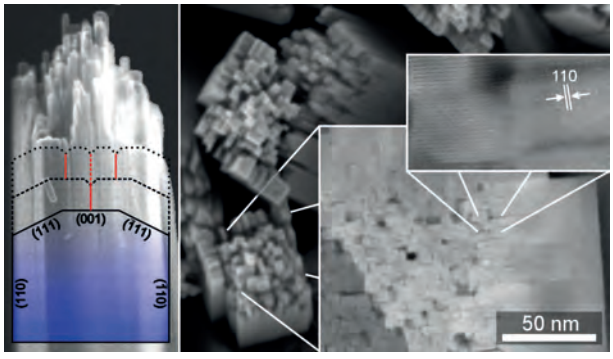


Fig. 3: *Secondary electron STEM image (left), top-view SEM image (middle), cross-section STEM images (right) of a hydrothermally grown TiO_2 nanowire. The nanowire has a faceted morphology with individual fingers at the top. Figure taken from [1]. The (110) lattice spacing in TiO_2 is 0.32 nm.*

shape within the nanowires by electron tomography is planned, in order to develop models of how they form and to detect possible oxidation state changes of the Ti ions at the surface/defects using EELS. The equilibrium shape as well as the surface structure will be analyzed in cooperation with the department of Computational Materials Design (CM). To further reduce the recombination, e.g. Nb_2O_5 core shell structures will be fabricated.

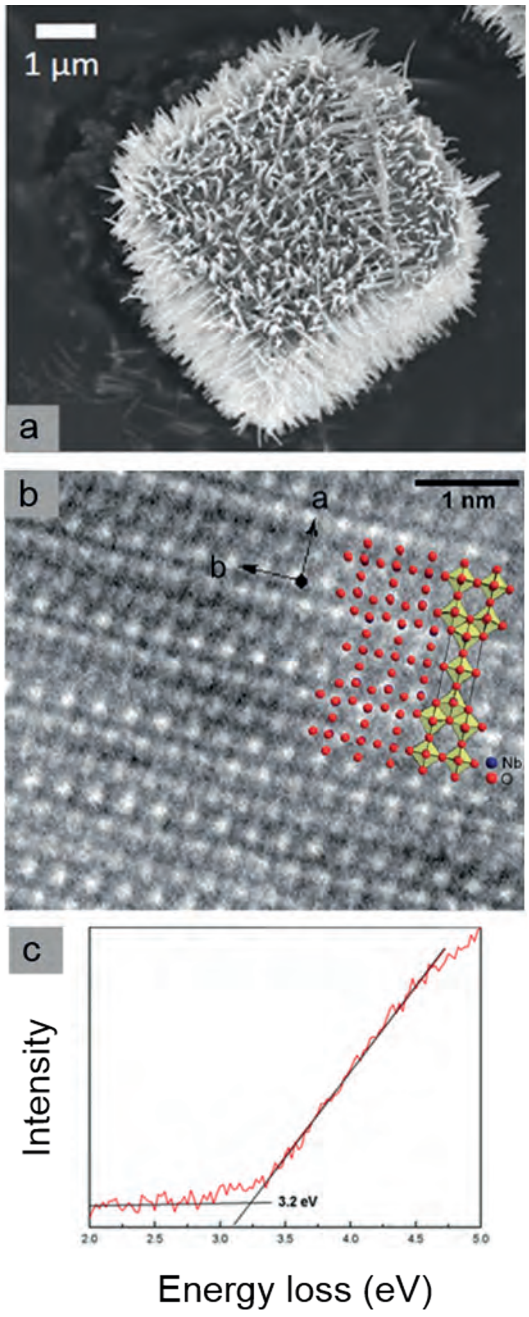


Fig. 4: *SEM image (a) of a $Nb_3O_7(OH)$ cube grown hydrothermally without a template consisting of a network of individual nanowires. (b) STEM image of a nanowire with indicated Nb and O positions in blue and red, respectively and (c) low loss spectrum to determine locally the land band gap. All images taken from [2].*

In general, Nb_2O_5 as well as $Nb_3O_7(OH)$ compounds can be considered as alternative materials for replacing TiO_2. They possess a high chemical stability and a similar band gap of about 3.1-3.2 eV like TiO_2. Besides the band gap, the energetic position of the upper valence and lower conduction band level is important for application as electrode material or electro-catalyst in energy and fuel generating devices. First experiments indicate suitable band positions for both compounds. We developed a one-step, template-free hydrothermal synthesis approach which allows us to grow crystalline $Nb_3O_7(OH)$ superstructures at low temperatures of 200°C [2]. The superstructures form cubes which consist of hierarchically ordered 3D nanowire networks (Fig. 4). X-ray- and electron diffraction analyses revealed that the individual nanowires forming the 3D network are single crystalline $Nb_3O_7(OH)$ with <010> growth direction (Fig. 4). The width of the nanowires is ranging from 10 to 50 nm and can be controlled by the synthesis conditions. The band gap determined globally using UV-Vis and locally in the TEM using low loss EELS revealed a value of 3.2 eV. The analysis of the ELNES of the Nb-$N_{2,3}$ and O-K edge indicate a nominal oxidation state of +5 of the Nb ions [2]. First photo-catalytic experiments conducted by our project partner Prof. Bettina Lotsch (MPI for Solid State Research, Stuttgart, and Ludwig-Maximilians Universität (LMU), Munich) and her team indicate that they are promising electro-catalyst for producing hydrogen fuel. In addition, the mechanical stability of the $Nb_3O_7(OH)$ cubes and individual nanowires will be investigated in close cooperation with the department of Structure and Nano-/Micromechanics of Materials (SN). This information enables us to estimate how we can use them e.g. as paste for different applications while maintaining their electronic properties.

The NG also participates in the DFG priority programme 1613 “Fuels Produced Regeneratively Through Light-Driven Water Splitting: Clarification of the Elemental Processes Involved and Prospects for Implementation in Technological Concepts”. Together with our project partners we strive to develop novel metal oxide photoabsorbers and synthesize them in different nanomorphologies to achieve efficient electrochemical and photoelectrochemical water splitting. The selection of viable material candidates is assisted by the group of Prof. Rossitza Pentcheva (University of Duisburg-Essen) via density-functional theory (DFT) calculations, synthesis and photo-electrochemical characterization are performed by the groups of Prof. Thomas Bein and Prof. Dina Fattakhova-Rohlfing (both LMU Munich) and we contribute by in-depth TEM and focused-ion beam (FIB) studies. In the first funding period, we focused heavily on improving hematite (Fe_2O_3) as a photoanode material. In an initial experiment we optimized a nanostructured hematite absorber layer

by Sn-doping [18] and found a strong increase in the rate constant for water oxidation. TEM investigations revealed an enrichment of Sn at the surface of the individual Fe_2O_3 nanoparticles, which is most likely responsible for improving the catalysis taking place at the surface. For the first time, this study showed that selective surface doping can have a catalytic effect in hematite photoabsorbers. We also worked on developing hierarchical systems consisting of an absorber layer and a highly conductive macroporous scaffold. Synthesis strategies were developed to fabricate novel macroporous transparent conducting oxide (TCO) scaffolds with excellent electron transport properties [19]. The latter is related to the formation of a continuous crystalline network, which was investigated by TEM. Due to the insight obtained during these studies, we successfully designed effective hierarchical systems consisting of a macroporous, conducting TCO scaffold (antimony-doped tin oxide) infiltrated with a Sn-doped Fe_2O_3 absorber layer [20]. Another strategy is to improve catalysis by ultrasmall Co_3O_4 nanocrystals which are homogenously distributed on the surface of the mesoporous Fe_2O_3 absorber layers [21].

Materials for Fuel Cells

Besides materials for photovoltaic devices and (photo)-electrochemical cells, we are also involved in material development and understanding of degradation processes in fuel cells. These research activities are done in close cooperation with our industry partner and are funded by the BMWi (Federal Ministry of Economics and Technology). Fuel cells convert chemical energy of a fuel into electrical energy via catalyzed redox-reactions on electrodes. They are environmentally friendly as during operation only water and heat are produced and a high efficiency is typically achieved which outperforms conventional power plants. However, fuel cells have the disadvantage of high production cost mostly due to the use of expensive catalyst materials and degradation phenomena which limit their lifetime.

We are working on high-temperature polymer electrolyte membrane fuel cells (HT-PEMFCs), where a polybenzimidazole (PBI) -based membrane is acting as proton conducting electrolyte and separating the adjacent anode and cathode from each other. The aim is to establish an understanding of excellent materials performance coupled with a high stability and low degradation rate. To achieve that goal, we analyze the microstructure of the different components before and after operation in detail to uncover the processes occurring during degradation. With this information at hand, we modify individual components as well as the whole fuel cell stack. In the case of the PBI-based membrane we found that longer thermal post-curing times lead to reduced degradation due to a change in the ordering of the polymer chains [22]. We also investigated the effect of adding silica nanoparticles to the membrane and observed an increase in stability due to the presence of the nanoparticles [23]. Detailed EDS and EELS studies of membranes containing differently sized nanoparticles revealed that they are homogenously distributed and consist of amorphous silica [24]. In experiments together with Prof. Viktor Hacker (Graz University of Technology), we investigated the long-term behaviour of platinum cobalt catalysts and found that they have a similar performance like the more expensive pure platinum catalysts [25]. We also replaced the anode carbon support material by tungsten oxide and investigated the performance and degradation behaviour after different operation times and modes including start-stop-cycles [26]. We found three dimensional networks of few nanometre thin, crystalline Pt rods on the WO_{3-x} grains with a size of up to about 1 µm after the deposition (Fig. 5). These rods decrease in size during operation and Pt is diffusing into different areas of the fuel cells, including the membrane [26]. Nevertheless, the degradation rate of the fuel cells containing the WO_{3-x} based anode was found to be lower compared to fuel cells using the standard carbon based anodes. In future experiments, we plan to study different noble metals

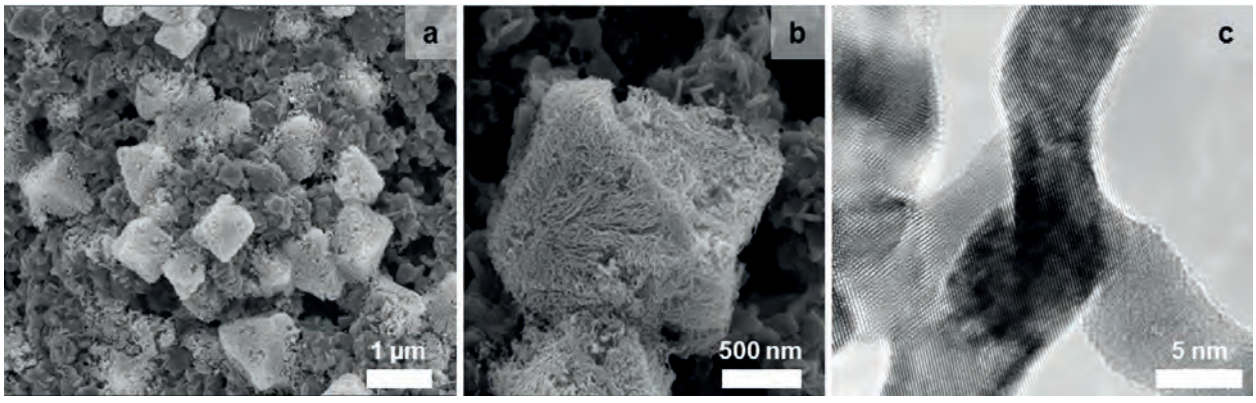


Fig. 5: *SEM images (a,b) of Pt networks on WO_{3-x} anode support materials. The network consist of Pt nanorods with a few nanometer in diameter. The deposition of Pt is described in detail in [26].*

and alloys as catalyst, and different high surface area carbon materials as well as various transition metal oxides as catalyst support material. These studies will be in close collaboration with the GO. In addition, we want to understand the growth of the Pt networks on the WO_{3-x} grains and will investigate different growth regimes.

Thin Films

As outlined, many of the nanostructures we investigate are prepared by wet-chemical synthesis protocols. Another approach we are working on is nanostructuring induced by controlled solid-state dewetting of thin metallic films. This project is done in close collaboration with the SN. In a first step, we grow epitaxial metallic Al films on single-crystalline Al_2O_3 substrates using molecular beam epitaxy and then perform annealing experiments using different conditions by varying the atmosphere, dwell times and annealing temperatures. FIB sectioning and TEM studies revealed that drum-like voids covered by a thin oxide layer which form during solid-state dewetting. Although the experiments were performed at only 600°C, single crystalline sapphire ridges form at the Al/sapphire interface (Fig. 6). The thickness of the Al film increases locally in this region of the sapphire ridge compared to the original film thickness. The forces involved in the dewetting process will be evaluated in collaboration with the CM. Future studies will concentrate on the determination of the grain boundary structure, since preliminary experiments indicate that specific grain boundaries are acting as nucleation sites of dewetting. Also here, a close link to the CM is given, since DFT calculations provide a detailed understanding of grain boundary structure and energy. The thermal stability and dewetting studies are also relevant for thin films in general, since this causes major problems for applications as conductive lines or protective coatings. Together with the SN and the newly established Max Planck Fellow group of Prof. Jochen Schneider (see p. 21) we investigate thin Mo_2BC thin films on Si substrates with the aim to understand the microstructural evolution during annealing. As grown, these films are amorphous and are then transformed to a nanocrystalline state when thermally treated. Preliminary experiments conducted with the GO demonstrated that they can also be used as electrodes in water-splitting devices.

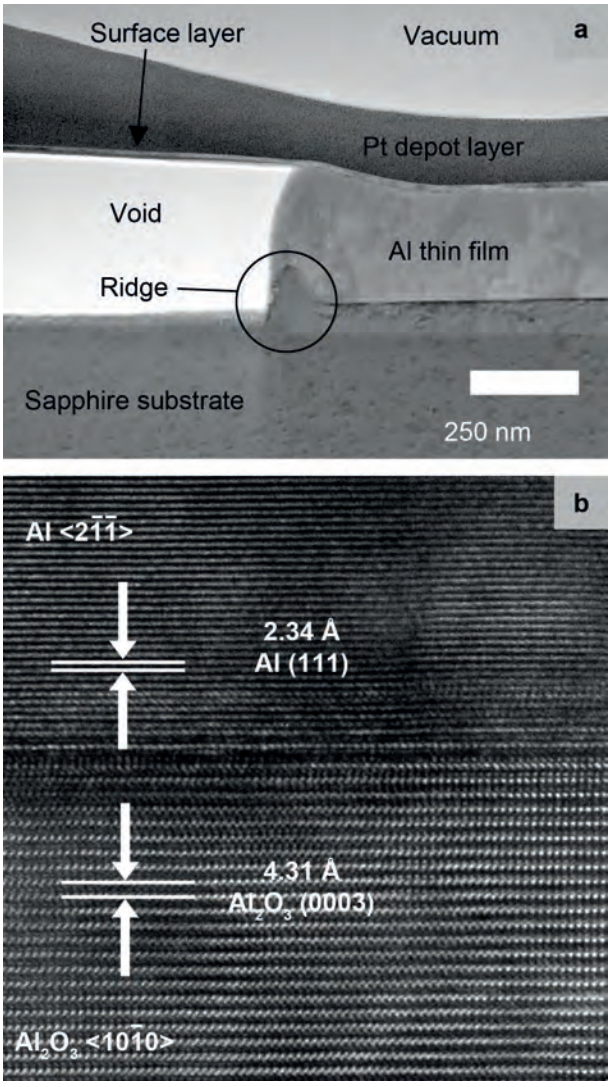


Fig. 6: *(a) STEM image of a FIB cross-section showing the formation of a drum-like void and ridge after solid-state dewetting of a thin epitaxial Al film on a single crystalline Al_2O_3 substrate. (b) HRTEM micrograph of the Al/Al_2O_3 interface marked in (b) indicating a low-index orientation relationship.*

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Research Projects in Progress

Betzler, Scheu (in collaboration with B. Lotsch*, L. Schmidt-Mende**, J. Ciston***, U. Dahmen*** (*LMU Munich and MPI for Solid State Research, **University of Konstanz, ***National Center for Electron Microscopy, USA)): In-depth investigation of novel 3D niobium oxide superstructures

Folger, Scheu (in collaboration with A. Wisnet*, A: Hartschuh*, L. Schmidt-Mende** (*LMU Munich, **University of Konstanz)): Synthesis and characterization of TiO_2 nanowires for electrochemical applications and solar cells

Frank, Scheu: Chalcopyrite nanomaterials for renewable energy applications

Gleich, Scheu (in collaboration with G. Dehm*, S. Djaziri*, J. Schneider** (*SN, **RWTH Aachen)): Characterization of nanolaminated materials by electron microscopy

Hengge, Scheu (in collaboration with Elcore, Munich): Structural and spectroscopic investigation of polymer based fuel cells

Hieke, Scheu (in collaboration in collaboration with G. Dehm, SN): From thin films to nanostructures

Müller, Scheu (in collaboration with T. Bein*, D. Fattakhova-Rohlfing*, I. Kondofersky*, J. Feckl*, A. Hufnagel*, R. Pentcheva** (*LMU Munich, **University of Duisburg): Investigation of photo-electrochemical water splitting-active nanostructures

Scheu (in collaboration with J. Mayer* (*RWTH Aachen)): Microstructure characterization – local structure, defect and chemical analysis (SFB 761/3 partial project C01)

Scheu (in collaboration with R. Hoffmann*, G. Langer**, C. Kirchlechner***, N. J. Balila*** (*LMU Munich, **Cambridge University; *** SN)): Morphology of Emiliania huxleyi coccospheres and effect on mechanical properties

Scheu (in collaboration with D. Raabe*, O. Cojocaru-Miredin** (*MA, **RWTH Aachen): Microstructural and spectroscopic analysis of thermoelectrics

Max Planck Fellow Group on Self-Reporting Materials

Group Head: J. M. Schneider

MATERIALS CHEMISTRY | RWTH AACHEN UNIVERSITY

Future technology challenges will no longer be simply addressed by today's material and processing solutions, which are often based on trial and error. Instead guidance will be attained from correlative experimental and theoretical research bridging all length scales. It is e.g. evident that future engineering components will be made of materials that are self reporting. Self-reporting materials "communicate" damage of the material via changes of properties that can be measured in service as a consequence of chemical changes on the atomic length scale and/or phase transformations. Harnessing this would provide invaluable functionality for damage assessment and control and would constitute a major leap forward as the "health" of any material component exposed to mechanical loads could be monitored in service. This fascinating basic materials science with tremendous technological implications is the focus of Schneider's Max Planck Fellow Group. Established in October 2015, the group will synthesize and characterize charge density modulated materials (multilayers & nanolaminates) regarding their elastic and plastic properties as well as their thermal and chemical stability. Based on these investigations and guidance from quantum mechanical calculations the charge density modulated materials with self reporting capabilities will be designed by substitution and/or addition of elements.

Thin film architectures with modulated charge density distributions will be grown by combinatorial vapour phase condensation as depicted in Fig. 1 (right). In a collaborative effort between the department Microstructure Physics and Alloy Design (MA) and Schneider it was demonstrated that the in Aachen grown multi-layered thin film architectures, shown in Fig. 1 (left) serve as model systems for the investigation of plasticity [1].

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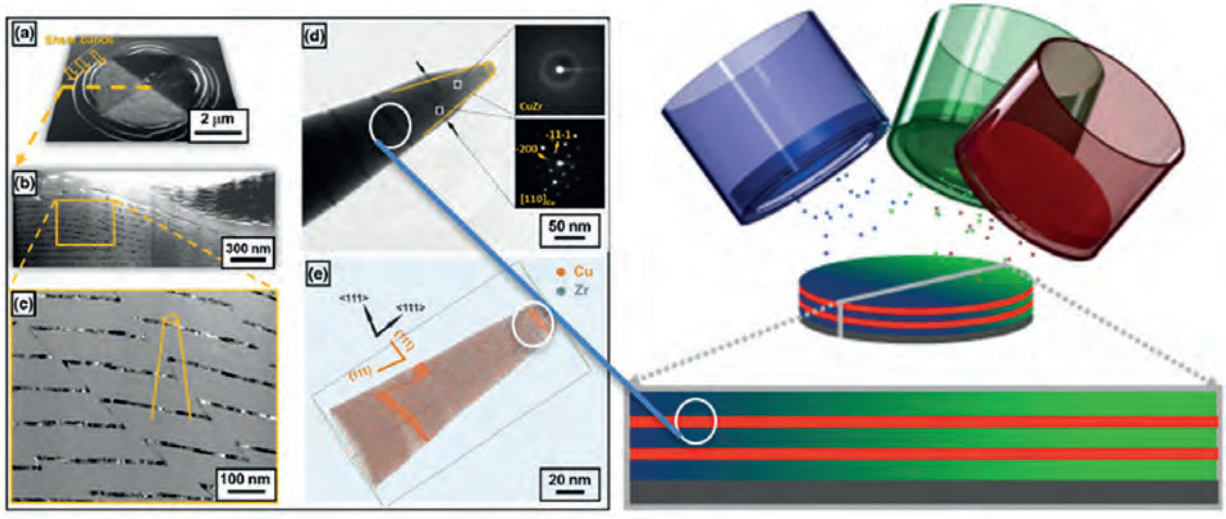

Fig. 1: *Illustration of the combinatorial synthesis approach to be employed in the Fellow group for the multilayers and nanolaminates (right). The colour gradient indicates a gradient in chemical composition [1]. On the left the images a-e show a plastically deformed crystalline-amorphous nanolaminate. Similar coating architectures will be utilized as initial platform to study the fundamentals of self-reporting materials.*

New Research Groups

Nanotribology

Group Head: S. Brinckmann

Department of Structure and Nano-/ Micromechanics of Materials (SN)

The mission of the group, which was established in December 2014, is to promote the understanding of tribology-formed microstructures including mechanical and chemical dominated layers and deformation on the nanometer scale. Initially, the focus is laid on the mechanical properties: plasticity, crack formation and growth, and the friction coefficient. We will study the dependence of the friction coefficient on the grain orientation and on secondary phases as well as on lubrication. Moreover, the tribology-induced microstructure evolution, i.e. grain refinement, grain re-orientation, as shown in Fig. 1, is a central theme of the group.

We will concentrate on the deformation of and due to microasperities, which resemble microstructural roughness that exists even on polished surfaces. Thereby, the research group will bridge the gap between conventional and atomistic tribology. Conventional tribology on the millimeter scale uses tribometers (e.g. pin-on-disk, disc-on-disc) to study friction & wear. As such, conventional tribology mimics the tribological deformation on the macroscale and includes all tribological mechanisms that interact with each other. Atomistic tribology uses the atom force microscopy (AFM) to scratch and image the surface, which resembles the deformation due to nanometer atomistic asperities. This atomistic roughness exists on any surface and leads to predominantly elastic deformation. By using the influence of the atomistic scale and focusing on the tribology of the nanometer scale, we can study fundamentally the individual mechanisms that occur on the macroscale.

A central benefit of the nanotribology is the ability to perform high throughput experiments (Fig. 2) using the same asperity, the same metal phase, the same lubricant and varying the friction power density, i.e. normal force and scratch velocity, over five orders of magnitude. Moreover, by varying the counter asperity radius and/or material, only small domains are required. Post-deformation inspection by AFM and scanning electron microscopy (SEM) allows us to quantify surface roughness, local grain re-orientation, grain sizes, cracks (Fig. 1) and allows determining the influence of the friction power density.

In the future, the investigation of the chemical mechanisms of tribology will move more into the focus. We have constructed an electro-chemical cell for the nanoindenter that allows studying hydrogen embrittlement (see p. 31). In engineering applications, the outer surface layers are dominated by chemical processes, which result in a 10 to 100 nm thick layer of sulfides, oxides and phosphates. If these outer surface layers are optimal, they result in ultra-mild wear rates, which are not measurable during state-of-the-art macroscale tribometer experiments. The nanotribology allows to separate the tribology mechanisms and to study the creation and growth of the surface layers individually and localized.

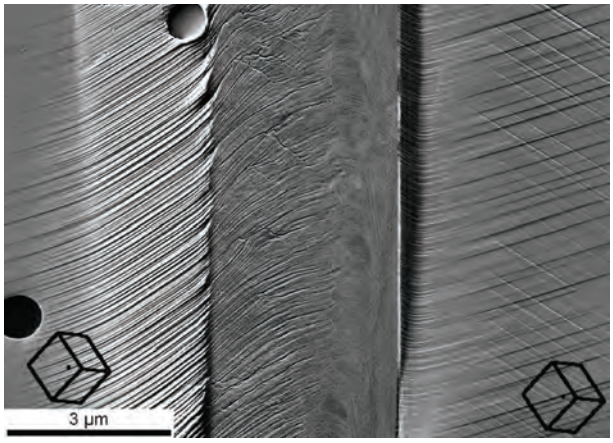

Fig. 1: *Surface steps on the sides of a scratch that runs through a large grain of austenite. Although scratching is a symmetric loading and both sides have the same crystal orientation, the plastic deformation and the surface steps are non-symmetric. On the right-hand side, two slip systems have the same activity, while on the left-hand side one slip system dominates plasticity.*

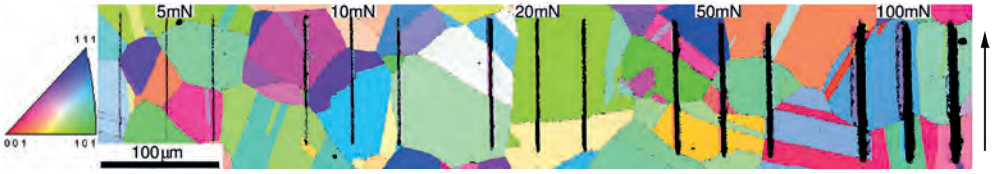

Fig. 2: *Electron-Backscatter-Diffraction (EBSD) image of the scratched area. The normal direction grain orientation is encoded as shown on the left-hand side. The scratch direction is shown on the right hand side. The local grain orientation in the scratch proximity is disturbed by the deformation.*

Interface Design in Solar Cells

Group Head: O. Cojocaru-Mirédin

Department of Microstructure Physics and Alloy Design (MA)

This new research group was established in 2013 with the support of the 'Bundesministerium für Bildung und Forschung' (BMBF NanoMatFutur competition). The mission of this group is to optimize solar cell efficiency based on an improved understanding of the relationships between chemical, structural, and electrical properties at the atomic-scale.

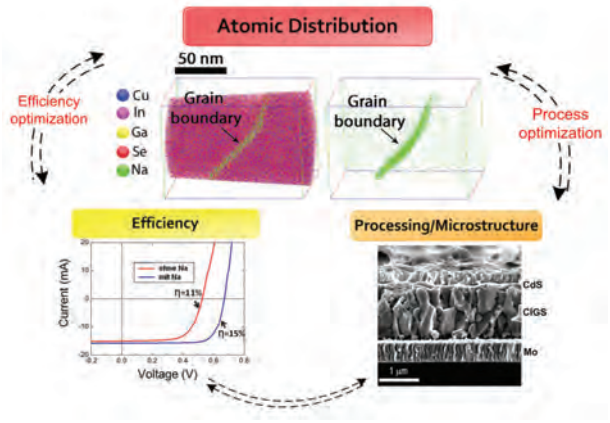

Fig. 1: *The correlation between Processing/Microstructure, Efficiency and Atomic Distribution for a Cu(In,Ga)Se_2 – thin film solar cell.*

During the past decade, designing new and beneficial internal interfaces in such photovoltaic materials has become crucial for controlling solar cell efficiency. Further improvements depend on a better understanding of the underlying atomic-scale interface mechanisms. A suited approach lies in mapping the cell's nanostructures by atom probe tomography for identifying the elemental distribution and the associated interface phenomena. Examples are impurity segregation at grain boundaries or p-n junctions as well as clustering and diffusion effects.

The research group concentrates on crystalline silicon [1] as well as on Cu(In,Ga)Se_2 and $Cu_2ZnSnSe_4$ thin-film [2] solar cells owing to their relatively high efficiency. To further establish c-Si and thin-film technology in this field both, the reduction in production costs and the enhancement of solar cell efficiency are essential. The latter aspect depends strongly on the internal interfaces as they can affect the transport of the photogenerated charge carriers. Moreover, the internal interfaces, such as grain boundaries and p-n junctions, are very often decorated by impurities which can profoundly affect cell efficiency [3], [4]. Fig. 1 illustrates that the efficiency of a Cu(In,Ga)Se_2 solar cell has been improved by almost 50% by merely adding minor amounts of Na (~ 0.1 at.%) to the absorber layer. Furthermore, Fig. 1 reveals that this increase in efficiency can be directly linked with Na segregation at the Cu(In,Ga)Se_2 grain-boundaries.

Therefore, the aim of this research group is to perform chemical, structural, and electrical characterization of the internal interfaces in solar cells by using latest nanometrology approaches, such as atom probe tomography in conjunction with complementary techniques such as electron backscatter diffraction, transmission electron microscopy, cathodoluminiscence, and electron-beam induced current. The overarching goal is then to synthesize novel and improved multicrystalline Si and Cu(In,Ga) Se2 or $Cu_2ZnSnSe_4$ thin-film solar cells in direct collaboration with several institutes at the forefront of solar innovation.

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TIME-BRIDGE: Time-scale Bridging Potentials for Realistic Molecular Dynamics Simulations

Group Head: B. Grabowski

Department of Computational Materials Design (CM)

The European Research Council (ERC) rewards the most prestigious and competitive scientific funding in Europe. The criterion for selection is scientific excellence. In 2015, Dr. B. Grabowski was awarded an 'ERC Starting Research Grant' for his innovative project proposal: TIME-BRIDGE: Time-scale bridging potentials for realistic molecular dynamics simulations.

The main objective of the recently established independent group entitled TIME-BRIDGE is to address the time scale problem encountered in molecular dynamics simulations. This problem originates in the fast thermal motion of atoms which happens on a femtosecond time scale. The processes determining relevant materials properties, such as dislocation motion, are instead taking place on significantly longer time scales, sometimes even in the range of seconds. Therefore, a gap of many orders of magnitude needs to be bridged.

Within TIME-BRIDGE, the key idea to solve the time scale problem is based on the pseudopotential concept. This concept is well known in the field of electronic structure theory where it helps to resolve the problem of highly localized core electrons. In TIME-BRIDGE a pseudo-potential will be developed that projects out the fast thermal vibrations of atoms allowing therefore to capture the relevant processes on large time scales. A core ingredient will be the quasiharmonic dynamical matrix which provides analytic solutions to the motion of atoms over arbitrary time scales.

Processes that will be studied using the new methodology will for example include nanopillar compression tests (Fig. 1). Such tests provide highly valuable information about the behaviour and interaction of the fundamental objects of plastic deformation. The performed simulations will be supported by complementary experimental measurements which will allow to carefully evaluate the developed techniques.

The TIME-BRIDGE project has a horizon of five years. Over this period, the funding covers three post docs, and a senior scientist. Dr. Grabowski and two post docs will be working on the theoretical developments and applications. One post doc will be performing the experimental measurements under the supervision of Dr. Kirchlechner from the department of Structure and Nano-/Micromechanics of Materials.

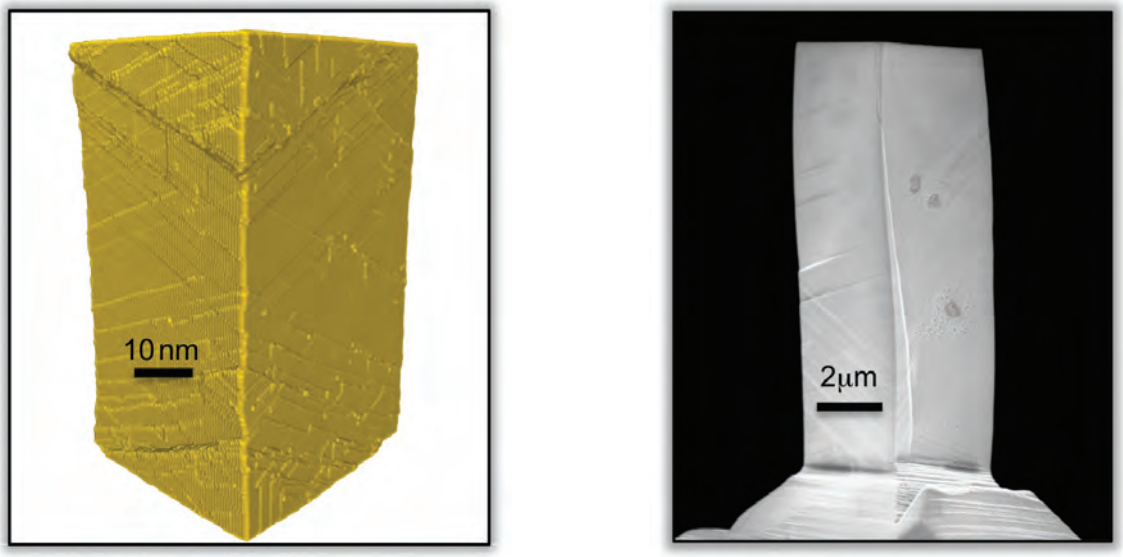

Fig. 1: *The left figure shows a theoretical simulation of a nanopillar exposed to a compression leading to characteristic deformation lines on the surfaces. The right figure shows an analogous experiment monitored under a scanning electron microscope. So far the theoretical and experimental results cannot be fully matched. The developments within TIME-BRIDGE will provide the necessary tools and knowledge to tackle the challenge.*

Alloys for Additive Manufacturing

Group Head: E. A. Jägle

Department of Microstructure Physics and Alloy Design (MA)

In April 2015, a new non-permanent research group has been established working on alloys and alloy design for Additive Manufacturing.

Additive Manufacturing (AM) is a rapidly maturing technology capable of producing highly complex parts directly from a computer file and raw material powders. It is different from conventional manufacturing methods in that the parts are produced additively, layer by layer, from raw material (e.g. powder, wire, liquid) until the desired shape is reached, as opposed to subtractive, e.g. by milling away material from a block of metal. Currently, AM is being adopted in more and more industries, specifically in aerospace, automotive, energy and (bio-) medical branches, and is being applied to produce an increasing number of diverse and highly complex products. This may lead to a revolution in manufacturing: The disruptive potential of AM lies in its ability to manufacture customised products with individualisation, complexity and weight reduction for free.

The first focus of the research group is to work on one of the central questions of materials science: How does the manufacturing process, in this case Laser Additive Manufacturing (LAM), influence the micro- and nanostructures of the employed alloys and hence their final properties? The group will not focus on the additive manufacturing process as such, but rather on its consequences to the material. For example, the rapid cooling and cyclic re-heating experienced by a part produced by LAM has an influence on the solidification behaviour of the material, introduces unwanted residual stresses (which can even lead to failure of the material) and can also trigger solid-state phase transformations.

Ultimately, the goal is not only to understand the peculiarities of the LAM process and its influence on the materials, but also to optimize existing materials and to design new, tailored materials. Since the existing materials that are in use today in the LAM processes have originally been developed for other processing routes, it is to be expected that their composition is not the optimum one for LAM. For example, the hot cracking behaviour seen in Ni-base superalloys produced by SLM might be alleviated already by small changes in the alloy composition that influence the grain boundary liquid film during the last stages of solidification.

Design of completely new alloys for LAM is so far almost entirely missing in the research landscape. The established alloys currently in use do not exploit the enormous opportunities inherent in this technique at all, leaving a profound gap towards its further development. In the research project “Advanced Alloy and Process Design for Laser Additive Manufacturing” (grant awarded by the research alliance between the Fraunhofer Society and the Max Planck Society), the project partners from MPIE and the Fraunhofer Institute for Laser Technology (ILT) are collaborating to develop tailor made alloys exploiting the unique characteristics of the LAM processes in combination with an adaptation of process engineering and process parameters to achieve alloy composition and properties *in-situ*. This can only be achieved by combining the expertise of the partnering institutes in the fields of alloy design and characterisation (MPIE) as well as process design and engineering (ILT).

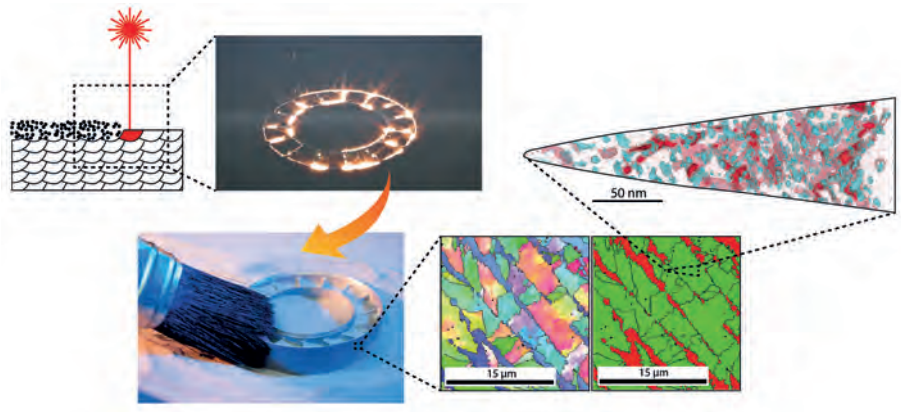

Fig. 1: *Schematic depiction of the layer-by-layer build up of a part by a Laser Additive Manufacturing process (specifically: Selective Laser Melting), together with Electron Backscatter Diffraction phase map (green: ferrite, red: austenite) and orientation map showing the microstructure induced by solidification and an Atom Probe Tomography map showing the nano-structure induced by heat treatment (light/dark red: 10% / 24% Mo isoconcentration surface, teal: Ti/Mo=1 isoatomic-ratio surface). The material under consideration is 18Ni-300, a maraging steel (1.2709).*

Nano-/Micromechanics of Materials

Group Head: C. Kirchlechner

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Designing future´s materials requires detailed knowledge of the fundamental mechanical properties across all length scales. But during macroscopic testing – i.e. in bulk samples – important details and mechanisms at the microstructural length scale remain unknown as they are being blurred by the collective behaviour and interplay in a complex microstructure. Recent advances in producing and deforming miniaturized mechanical samples, site-specific with yet unreached small dimensions, bring the former vision of closely following materials behaviour at the outmost important length scales into reality.

Fig. 1: *Example of compressed copper micro pillars. The pillars in (a,c) are single crystalline with clear slip steps through the entire pillar documenting free glide of dislocations. The centered pillar (b) is comprised from the two single crystalline ones at the side, with a grain boundary in the center. Many more faint slip steps document the important role of grain boundaries as obstacles for dislocation motion.*

The new research group Nano- and Micromechanics of Materials, which started in March 2013, is probing the mechanical properties regarding plasticity, fracture and fatigue at the micron and sub-micron scale. But the spirit of nano- and micromechanics surpasses being a mechanical microscope by far: A central aspect of the group is to interlink the mechanical response to the underlying and evolving defect structure, i.e. to measure and observe dislocation densities and interaction mechanisms, crack length, phase transformations and change of electrical properties *in situ* during mechanical loading. This is accomplished by advanced microstructural characterization tools in-house (e.g. transmission electron microscopy) or at a large-scale synchrotron facility (e.g. ESRF, BESSY II). The final goal of the group is to develop material models at the microstructural length scale serving as guidelines for materials development and input for materials simulations.

Two approaches are followed in our group: Thin film testing, where typically a rigid film is deposited on a compliant substrate and subsequently strained in a tensile device; and focused ion beam (FIB) based micromechanics, where test specimens being not too different from their large scale counterparts are produced in a FIB microscope and tested in a nano-indentation device (see “New Scientific Laboratories”).

Within the past years, the role of phase transformations on the adhesion and fracture properties of metastable face centered cubic cobalt thin films had been studied [1]. Furthermore, dislocation-grain boundary interaction mechanisms [2,3] as well as fatigue in pure copper in single crystals [4] and bicrystals had been investigated. The group hosts already 9 scientists and has established a strong network in Germany, Europe, the United States of America and Japan including several scientific industry collaborations.

In the future, high temperature capabilities will be built up to study e.g. brittle to ductile transition phenomena of engineering materials, high temperature properties of intermetallics and hard coatings.

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Advanced Transmission Electron Microscopy

Group Head: C. Liebscher

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Mission: The mission of the Advanced Transmission Electron Microscopy group revolves around the characterization and design of structural and functional materials from the atomic level to mesoscopic length scales. The group was established in April 2015 to link atomic resolution transmission electron microscopy (TEM) with novel *in situ* TEM techniques. From a materials perspective, key aspects are the investigation and development of interface dominated materials and the related interface structures and properties, the interplay of local atomic arrangements and the corresponding deformation behaviour and the design of novel nanostructured materials.

Atomic scale characterization: A core theme of the group is the length-scale bridging characterization of materials to establish a complete microstructural concept providing the basis for new material development. An example of such an approach is given in the figure below, where the arrangements of precipitate structures and their evolution is characterized from a mesoscopic scale down to the atomic level [1]. This approach enables a direct link to theoretical predictions on the basis of first-principles calculations of phase stabilities and interfacial phenomena. Aberration-corrected TEM plays the key role in determining the chemistry, bonding characteristics and crystallography with sub-nanometer resolution. Such advanced techniques require the development of new imaging and data processing schemes representing a further area of research. The coupling of atomic resolution imaging with atomistic simulations will be essential for modern and innovative material design and is therefore considered to be another core part of the group.

In-situ **microscopy:** The understanding of material behaviour on the nanoscale through *in situ* microscopy techniques will complement the atomic resolution characterization. The focus lies on *in situ* deformation and heating methods, since atomic arrangements are dictating the mechanical and thermodynamic properties of materials. The necessity for decoding the material behaviour under externally applied conditions is to have a full picture and control of the nanostructure of a material [2]. A fundamental correlation of atomic scale characterization and *in-situ* deformation studies is extending the research topics of the Advanced TEM group. The atomistic structure of segregation effects at interfaces – such as grain boundaries – and the respective nanoscale deformation behaviour will serve as paradigm for this novel, comprehensive approach.

Current activities: The ongoing research activities are focusing – but are not limited – on the characterization of nanocrystalline, metastable Cu-Cr alloys [3] and the respective bonding characteristics, the atomic structure and segregation behaviour of interstitial and substitutional elements at grain boundaries, the design and characterization of nanostructured materials with hierarchical microstructure [1] and the microstructural investigation of semiconducting nanowires.

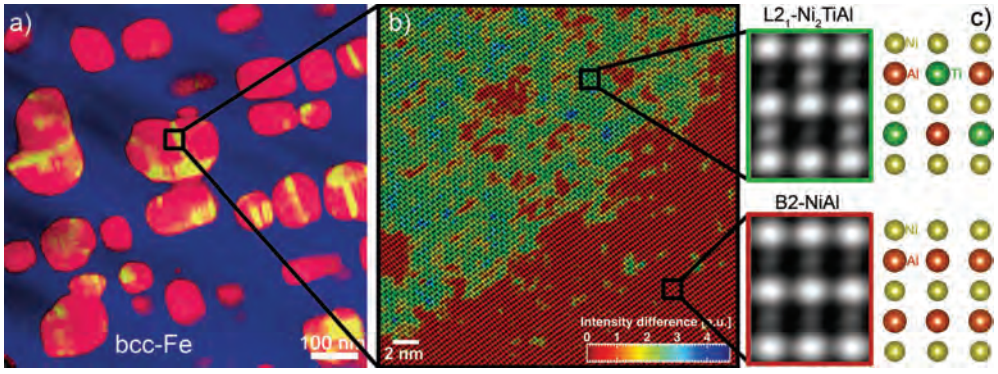

Fig. 1: a) *Hierarchical microstructure of a precipitation strengthened ferritic alloy with two-phase B2-NiAl / L2$_1$-Ni$_2$TiAl precipitates.* **b)** *Atomic resolution micrograph of a B2-L2$_1$ interface. The colouring scheme is based on the local order parameter of the B2- and L2$_1$-phases.* **c)** *Atomic arrangement of the B2-NiAl and L2$_1$-Ni$_2$TiAl phase with a schematic projection of the corresponding crystal structures.*

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Electrochemistry and Corrosion

Group Head: M. Todorova

Department of Computational Materials Design (CM)

The "Electrochemistry and Corrosion" group was established in October 2015 in the CM and is headed by Dr. Mira Todorova. The objective of the group is the development of quantum mechanics based multi-scale simulation techniques and their application to problems in electrochemistry, with a strong focus on corrosion. The activities in the group are tailored to provide in-depth insight into the functionality and evolution of materials properties under the influence of realistic environments. The thus gained understanding of experimental observations and the identification of relevant physical mechanisms will aid the development of strategies to counteract, retard or suppress degradation phenomena in materials.

The complexity of solid/liquid interfaces, which are at the core of most electrochemical processes of practical importance, presents a major challenge: all the obstacles faced in the context of the individual phases comprising such an interface come together and are further enhanced by the presence of spatially rapidly changing electric fields. For example, the statistical nature of liquids, translates into long sampling trajectories of molecular dynamic simulations. On the other hand, the nature of a solid electrode (metal or semiconductor/insulator), even in the most simple case where it can be described as a (defect free) model system, is of central importance in the context of the potential drop inherent to a solid/liquid interface, and usually translates in length scales which are beyond the extend of unit cells used in first-principles calculations. However, an accurate description of the electronic structure (of both solid and liquid), including the alignment of band structure and redox levels, is essential for understanding the mechanisms driving the involved reactions. While this list is not complete, it illustrates that a direct brute force quantum mechanical approach is unfeasible and well controlled approximations and efficient numerical formulations are of utmost importance.

A first -step in this direction was the development of an approach which links *ab initio* calculations quite naturally to experimental observables characterising and determining the state of an electrochemical system, such as the pH-scale and the electrode potential. The approach exploits the similarities between charged defects in semiconductors and ions in liquid, is based on a fully grand-canonical description of both ions and electrons, and unifies and "translates" concepts in semiconductor defect chemistry and electro-chemistry [1]. This approach provides a sound basis for our further developments which, on one hand, strive to benchmark, analyse and quantify the required and achievable accuracy of presently available *ab initio* techniques focusing on the calculations of ion solvation and, on the other hand, aims to identify mechanisms driving reactions, for example, the construction of defect stability phase diagrams which enable, e.g. to identify the point defects which are relevant in the context of oxide film growth (see p. 161).

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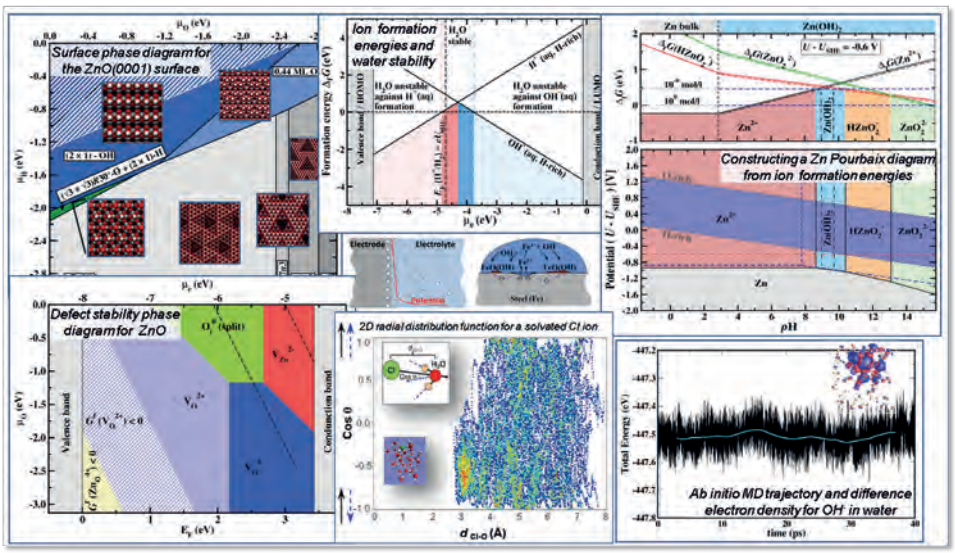

Fig. 1: *Sketch of current activities in the group, which include surface, interface and bulk stability with respect to the environment and native defects (Pourbaix and phase diagrams) and ions in water (2d radial distribution function, molecular dynamics trajectory).*

Atomistic Modelling

Group Head: S. Wippermann

Department of Interface Chemistry and Surface Engineering (GO)

This new *ab initio* theory group is located inside the otherwise exclusively experimental GO department and was established in February 2013. Additionally, in January 2014 the group leader Stefan Wippermann received a grant of 1.17 Mio. € from the German Federal Ministry for Education and Research (BMBF) within the NanoMatFutur competition to establish an independent junior research group for "Semiconducting Nanocomposites with Tailored Electronic and Optical Properties". This independent group will be incorporated into the Atomistic Modelling Group. We work in direct collaboration with experiment to gain insights into key processes at solid-solid and solid-liquid interfaces, nanostructures and in the gas phase, which are inaccessible by other means. Employing predictive *ab initio* modelling techniques based on density functional theory and beyond [1], we focus on the general fields of materials for solar and chemical energy conversion and storage.

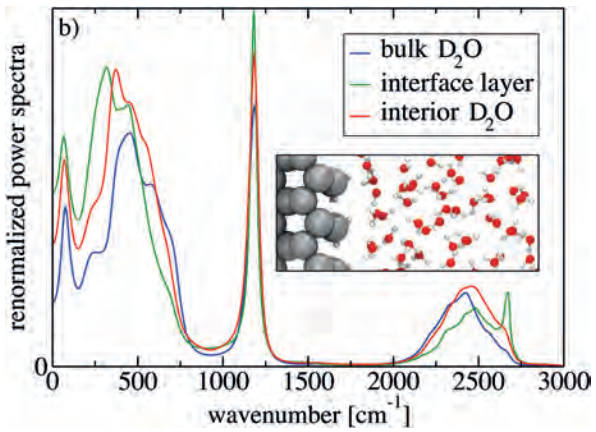

Fig. 1: *Vibrational power spectra of the deuterated Si(100)-D/D_2O interface, partitioned into contributions from bulk and interfacial water. A red-shift in the libration modes is observed compared to bulk water and a shoulder in the stretching modes of interfacial water, related to a breaking of the H-bond network.*

One particular research area is the combination of atomistic thermodynamics and theoretical spectroscopy. Many of the surface characterization and analysis techniques common to surface science under ultra high vacuum conditions are not applicable to solid-liquid and solid-solid interfaces. Techniques to probe such interfaces, most notably spectroscopy, are often very indirect. We employ atomistic thermodynamics to identify and predict relevant structural motifs and processes at interfaces. Performing *ab initio* calculations of, e.g., vibrational, optical excitation and electron paramagnetic resonance (EPR) spectra allows for direct comparison to experiment.

Solid-liquid electrode-electrolyte interfaces are of tremendous technological importance in fields as varied as, e.g., electrolysis and -catalysis, corrosion, batteries, fuel cells and solar water splitting devices. Often multiple interfaces are involved between metals, semiconducting metal-oxides and liquid water. In addition, ions solvated in the electrolyte screen the charge on the solid surface, forming an electrochemical double layer. A detailed understanding of such interfaces at the atomistic level has so far remained elusive. Significant challenges persist even in the *ab initio* description of the relevant bulk materials, e.g. transition metals and water. Therefore coupled theory-experimental investigations on well controlled and characterized systems and interfaces play a key role, in order to develop robust strategies to interpret experiments and validate theory. Starting from model interfaces, such as well-defined single-crystalline semiconductor-water interfaces, we investigate the atomistic and electronic structure of both the surface and the electrochemical double layer, thermodynamic stability, solvation of the surface, interaction with ions in the electrolyte, and the dependence on pH and the applied bias potential from first principles. One of our major scientific goals is to develop methods to predict the structure of electrochemical interfaces employing first principles atomistic thermodynamics, validate predicted structures against spectroscopic experiments and establish structure-property relationships.

Analogous considerations apply to complex nanometer-sized solid-solid interfaces, e.g. at surface-supported nanowires or nanocrystals embedded in a host matrix. Such nanocomposites are a promising approach to assemble functional materials with specifically designed electronic and optical properties, with potential applications as catalysts in electrochemistry, light absorbers for photovoltaics and light emitters in LEDs and lasers. Synthesis can be performed completely by inexpensive wet chemical solution processing. These nanomaterials may exhibit new functional properties not observed in conventional semiconductors, e.g. efficient carrier multiplication where an incoming photon creates more than one exciton [2,3]. The electronic and optical properties of these nanocomposites are dominated by interfaces and in particular defects at interfaces. We are systematically exploring the rich configurational space of technologically relevant nanocomposites. Subsequently, the obtained models are validated by means of joint theory-experimental IR, Raman and EPR spectroscopy. Such carefully developed models form an ideal basis to obtain key insights into their nanoscale physics and chemistry, allowing for a more rational device design.

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New Scientific Laboratories and Facilities

Micromechanics - Small Scale Testing Facilities

C. Kirchlechner

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Probing material properties at the micron scale requires dedicated machines and setups for sample manufacture, sample testing, and *in situ* as well as post mortem defect analysis. Within the past three years capabilities to produce and deform micron and submicron sized samples have been built up in the department Structure and Nano- /Micromechanics of Materials and are briefly summarized here.

The largest share of small scale samples at the MPIE is nowadays produced via a focused ion beam (FIB) based route, for which a Zeiss Auriga® Crossbeam system was installed in 2013. The FIB is operated with 5 keV to 30 keV Ga^+ ions focused typically to a beamsize in the range of some nanometres. In contrast to standard FIBs, the attached nano-patterning and visualization engine (NPVE, Fibics Inc, Ottawa, Canada) gives full access to the beam control. Thus, complex shapes with varying geometries requiring different dwell times locally can easily be set and manufactured in an automated way. By that, the NPVE helps us to surpass one of the bottle necks during micromechanical experiments: the manufacture of a statistically sound number of samples. Typical sample sizes produced via this route vary from several tens of nanometres up to 20 micrometres, which is in a size regime where a transition from a deterministic to a stochastic behaviour is observed, and therefore a high number of experiments is required.

On top of the dedicated sample manufacture, also testing rigs spanning over several orders of magnitude have been implemented in past years. Our indentation systems are either able to operate at a synchrotron beamline without obstructing the x-ray beam, are operated inside a scanning electron microscope (SEM), or in the transmission electron microscope (TEM). The variety of testable sample sizes ranges from some tens of nanometres (TEM, tested with Hysitron Pi 95 TEM Picoindenter®, Hysitron Inc., Minneapolis, USA) over several tens of micrometres (SEM, tested with ASMEC Unat II, Radeberg, Germany) to almost 500 µm (Laue diffraction, built at the MPIE). The various new loading rigs provide significant overlap in maximum force and strain rate and complement the existing (macroscopic) straining rigs at the MPIE. Thus, we are now able to probe material´s response from the low nanometre regime up to macroscopic sample and component dimensions, giving us the unique ability to understand the material´s behaviour across the relevant length scales.

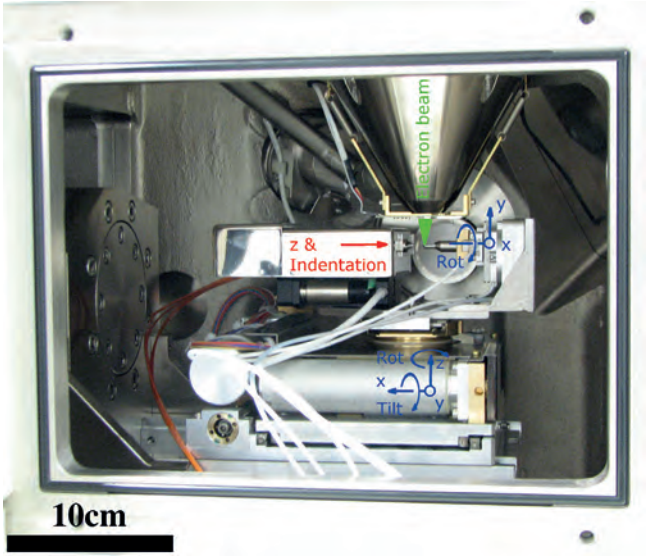

Fig. 1: *Asmec Unat II installed in a Jeol JSM 6490 SEM, our standard testing rig for micron-sized samples. The counterparty (e.g. a diamond or tungsten tip) is marked with "Indentation", with the sample support pin opposite of it. Sample and indenter can independently be moved along 4 axes with submicron resolution. In addition, the entire setup can be oriented with 5 additional axes, which allows for versatile experimental setups (Electron Backscatter Diffraction, ECCI).*

All of the newly installed machines are aimed for *in situ* operation – i.e. advanced characterization tools as for instance the electron contrast channelling imaging (ECCI as pioneered in the Microstructure Physics and Alloy Design department) or dedicated environmental loading conditions using a hydroelectric cell (in collaboration with the Interface Chemistry and Surface Engineering department) – and thus, are well suited for answering advanced questions in various material systems.

To increase the throughput of our testing facilities with additional environmental capabilities (e.g. gases, temperature), a chamber equipped with an optical microscope (Olympus DSX 500i) is being built within the next year.

Nanoindentation and -tribology Laboratory

J. Duarte-Correa, S. Brinckmann

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Tribology, i.e. friction and wear, depends significantly on five parameters: the material, the surface roughness, the counter material, lubricants and the environment. In engineering applications, boundary layers develop on the surfaces if the five parameters have been optimized and these layers consist of a chemically and a mechanically dominated zone. The former has a thickness on the order of tens of nanometer and the latter has a thickness on the order of micrometers. To reduce the friction, one has to reduce the adhesion of microasperities, which exist on any – even polished – surface. The study of adhesion, mechanical deformation, microstructure evolution, surface topology formation and the chemical processes surrounding tribology are at the center of the Nanoindentation and -tribology Laboratory (established June 2014).

In addition to the focus on tribology, the laboratory is set up to perform nanoindentation experiments, since both scientific research areas overlap. These nanoindentation experiments are either required for other research projects to extend the possibilities of the Institute or they set the basis of the deformation processes later extended to the lateral direction during tribology studies. Until recently, the nanoindentation experiments were limited to 10 mN at the Institute, which proved to be a limitation for very hard bulk materials and hard thin films. This limitation was especially detrimental for samples with a strong surface roughness.

The central equipment of this laboratory is the Keysight Nanoindenter G200 with a normal force range until 500 mN, which allows studying deformation even with blunt indentation tips. The normal force is applied with a coil-magnet assembly and the normal displacements are recorded by a capacitance gauge. In addition, the lateral forces in both directions are measured and the friction coefficient is evaluated. The transitional stage with nanometer lateral resolution allows targeting small phases during nanoindentation and micromechanical tests, and executing atomic force microscopy (AFM) like surface topology scanning prior and post deformation.

One key feature of the G200 is its ability for extensions. We constructed a three-electrode electrochemical cell that positions the sample immersed into the electrolyte below the indenter tip prior to the experiment. In addition, the cell allows for sample rotation and electrolyte exchange. The connected Gamry reference 600 potentiostat allows measuring and prescribing currents and voltages. Lubricants can be entered in the cell in a similar way. Supplementary, the G200 allows for the use of multiple indenter tips. Special long indenter tips are used to penetrate the samples immersed into the electrolyte. Conventional diamond tips are used in nanoindentation and nanotribology; here we constructed stainless steel tips to study the steel-on-steel contact and to better understand the five parameters of tribology.

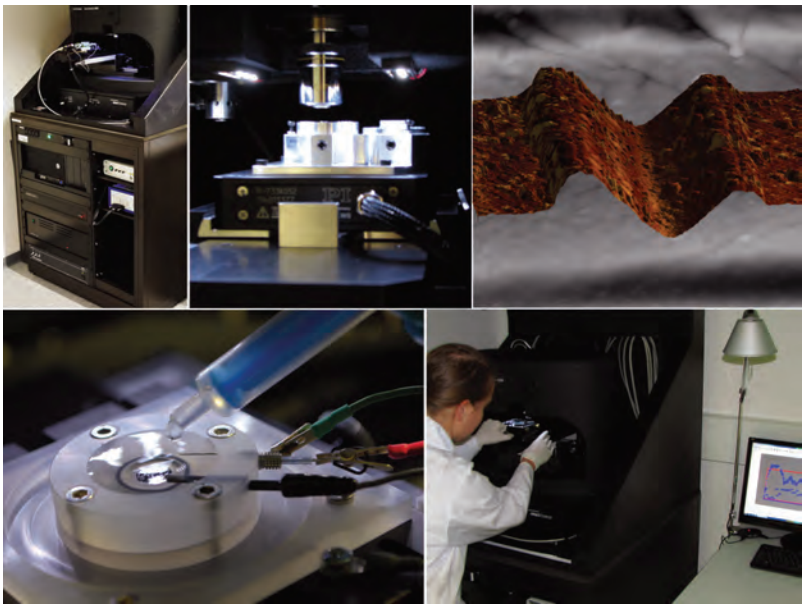

Fig. 1: *Snapshots from the Nanoindentation and -tribology Lab: Nanoindenter, nanometer stage, Atom Force Microscopy (AFM) image of a scratch in Cu, electrochemical cell and scratch experiments.*

Advanced Transmission Electron Microscopy Facility

C. Liebscher

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Introduction: Transmission electron microscopy (TEM) has a long history and tradition at the MPIE. In the past, the focus was on conventional microscopy, but also more advanced techniques such as scanning TEM (STEM), analytical and *in situ* microscopy became part of research. The Advanced Transmission Electron Microscopy Facility was established in May 2015 with the commission of an aberration-corrected (S)TEM. Correcting for lens aberrations is key to provide researchers with atomic resolution imaging and spectroscopy. The probe-corrected FEI Titan Themis 60-300 combines all state of the art (S)TEM and spectroscopic techniques with an emphasis on scanning transmission electron microscopy. The Advanced Transmission Electron Microscopy Facility will be complemented in mid 2016 by the installation of an image side corrected FEI Titan Themis. The (S)TEM facility enables atomic scale investigation of complex material systems, including interfacial phenomena and precipitate structures. The mission is to resolve the crystallographic structure, chemistry and bonding characteristics of materials developed at MPIE with atomic resolution.

(S)TEM facility: The microscope is equipped with a high-brightness electron source in combination with a Wiener-type monochromator. Reducing the energy spread (<0.2 eV) of the electrons is beneficial for special TEM imaging techniques and mainly for high-energy resolution electron energy loss spectroscopy (EELS). The 3-condenser system allows for nearly parallel illumination in TEM-mode and enables a flexible use of the monochromator in combination with STEM imaging. In STEM, the resolution is mainly limited by lens aberrations of the probe-forming condenser lens. The probe corrector allows for a correction of up to 5th order lens aberrations leading to a STEM point resolution of down to 70 pm. In total, seven STEM-detectors are available for bright-field (BF), annular BF (ABF) and annular dark-field (ADF) imaging. A windowless, four quadrant Silicon-Drift (SDD) EDS (Energy Dispersive Spectroscopy)-detector (FEI Super-X) with a solid angle of >0.7 sr enables atomic resolution chemical analysis, including light elements like oxygen and carbon. The monochromated electron gun facilitates a flexible adjustment of beam currents up to 2 nA necessary for analytical STEM. Electron energy loss spectroscopy (EELS) can be utilized in combination with TEM or STEM by the post-column energy filter Quantum ERS (Gatan). The integrated electrostatic shutter provides ultra fast acquisition of 1000 spectra/s and dual-channel EELS with simultaneous acquisition of low and core loss spectra. In addition to the CCD (Charge-Coupled Device) of the energy filter, the microscope is equipped with a 16-megapixel CMOS (Complementary Metal Oxide Silicon) camera for high quality, high-speed image acquisition. Precise sample positioning and drift correction is possible through a piezo controlled sample stage. For studying beam sensitive materials, the acceleration voltage can be reduced from 300 to 120 and 60 kV, maintaining sub-nanometer resolution. To overcome the projection problem in TEM, a high-tilt tomography holder with acquisition and reconstruction software is available. The figure illustrates the microscope column and two examples of atomic resolution STEM experiments on $SrTiO_3$ and a Si grain boundary.

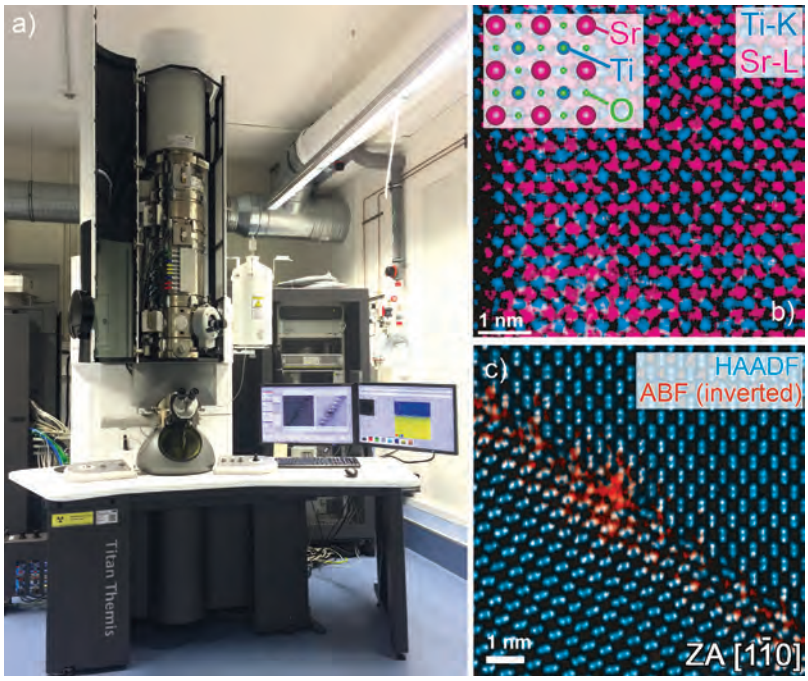

Fig. 1: a) *Microscope column of the Cs-probe corrected FEI Titan Themis 60-300 with highlighted features.* **b)** *Atomic resolution STEM-EDS elemental mapping of $SrTiO_3$.* **c)** *Composite image of simultaneously acquired high-angle annular dark-field (HAADF) and annular bright-field (ABF) STEM images of a ∑ 3{112} grain boundary extracted from a intentionally doped multicrystalline Silicon wafer (department of Microstructure Physics and Alloy Design).*

The Near Ambient Pressure Microfocus Photoemission Spectroscopy System

D. Vogel

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Chemical reactions at gas/solid and liquid/solid interfaces play a crucial role in many processes, from corrosion to catalysis. A fundamental in-depth understanding of the underlying mechanisms is difficult to obtain due to experimental restrictions for interfacial analysis. The Institute´s new near-ambient-pressure X-ray photoelectron spectrometer (NAP-XPS) bridges the pressure gap between UHV (ultra-high vacuum) and ambient pressure, and thus the material gap between simplified model systems investigated under low pressure conditions and complex real systems. Whereas NAP-XPS systems are well established as end stations at synchrotron facilities, our custom-made setup is a prototype of a new commercial laboratory-based system. It enables *in-situ* analysis of surface processes in a pressure range up to 40 mbar at temperatures up to 800°C in an exchangeable high pressure reaction cell with a very small volume.

Thus experiments can be carried out in highly reactive gas atmospheres without contaminating the UHV chambers or the analyser. XPS and UPS (ultraviolet photoelectron spectroscopy) measurements can be performed using either a monochromatic micro focusing X-ray source, a twin anode (Mg/Al) X-ray source or a small spot UV-source. The system is equipped with devices for sample cleaning, evaporation and characterization such as sputter guns, evaporators or LEED. Additional several bolt-on chambers are equipped to perform pre-treatments or pre-characterizations of the samples, such a high-pressure/high-temperature chamber, electrochemistry cells, or a chamber for performing Kelvin Probe measurements as well as Thermal Desorption Spectroscopy (TDS). The system and its bolt-on chambers are connected to a complex gas installation for cleaning (impurity level < 1ppb) or conditioning of the reaction gases (e.g. defined humidity). The complex installation covers all research fields of the department and offers customized solutions for the related individual projects.

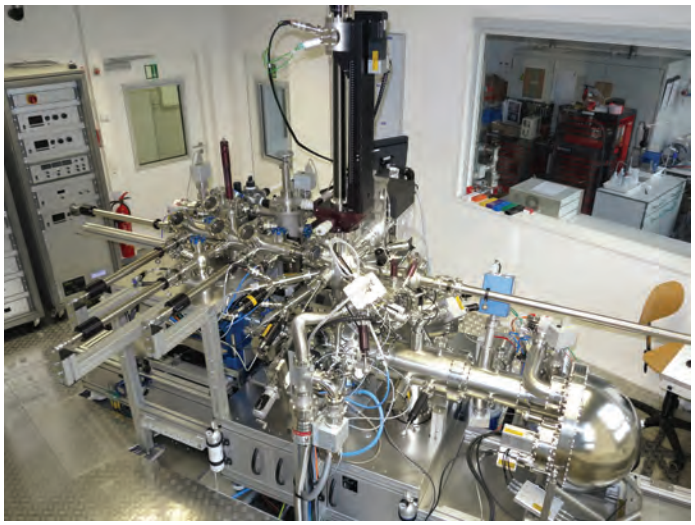

Fig. 1: *Photo of the NAP-XPS: The footprint of the system fits ideally into the laboratory, whereas all peripherical devices such as backing pumps, coolers and gas supply are installed in the neighboring technical room.*

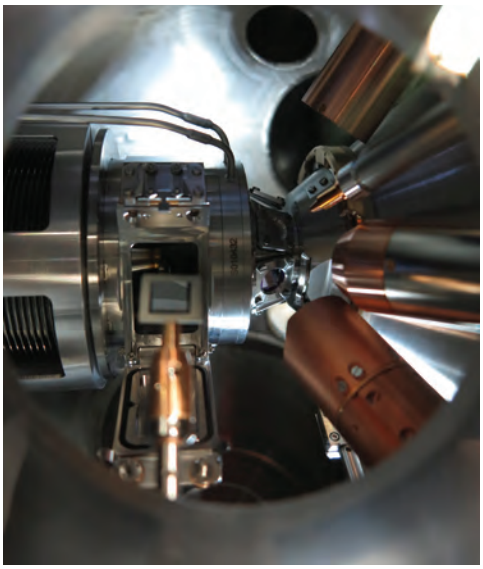

Fig. 2: *Photo of the reaction cell inside the UHV chamber: It is docked with the differentially pumped analyzer and opened for sample transfer.*

Long-term Oriented Method Development

Development of Electrochemical Water Based *in-situ* TEM and Potential- and Time-Dependent Study of Platinum Alloy Nanoparticle Dealloying

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Platinum is still the best choice for the use as an electrocatalyst in the state of the art proton exchange membrane fuel cell (PEM-FC) [1]. Although its properties and performance have been extensively studied in the last decades, still, its degradation processes in PEM-FC are not completely resolved. Recently, it has been shown that the main degradation mechanisms are Pt dissolution and carbon corrosion [2, 3]. These novel insights were only possible due to introduction of new advanced characterization techniques like identical location transmission electron microscopy (IL-TEM [4]) and scanning flow cell coupled to ICP-MS (inductively coupled plasma mass spectrometry) [3] all developed at the MPIE. In order to even further deepen our fundamental understanding especially of structural degradation of catalyst nanoparticles on supports, novel *in-situ* methods will have to be developed and explored.

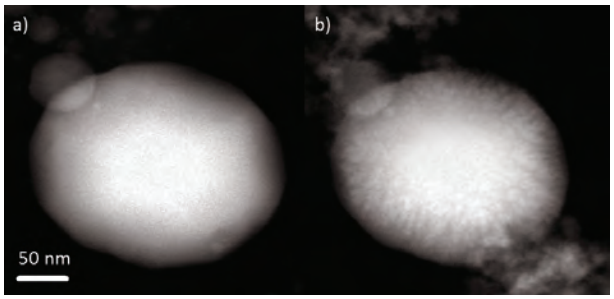

Fig. 1: *Electrochemical water based in-situ TEM before* **a)** *and after* **b)** *dealloying treatment of a $PtCu_3$ nanoparticle in 0.1 M $HClO_4$. Snapshots out of the in-situ video recorded of the dealloying of PtCu3 nanoparticles in 0.1 M $HClO_4$ and subsequent copper beam induced redeposition. The big particle is 200 nm in diameter.*

Bringing together the extensive expertise of the two departments particularly with regards to development of advanced characterization techniques, we plan to develop and utilize advanced electrochemical characterization *in-situ* water-based TEM technique, gaining valuable insights into potential- and time-dependent electrochemical processes occurring in materials for energy conversion in their native environment with nanometer resolution. It will enable us in future to obtain the necessary insights and breakthroughs related to for instance corrosion or dealloying of platinum based nanoparticles. We recently utilized a commercial holder for electron microscopy (Protochips Poseidon 510) and presented initial results on platinum alloy nanoparticle dealloying [5]. These experiments helped us to already expose some of the challenges and limits of the studied system, as for instance beam effects and resolution. Next steps include far-reaching *in-situ* experiments in alloy model systems and nanoparticulate catalysts, and we are confident that they will provide new, game-changing insights into fundamental processes on the nanoscale.

This research was supported by a Marie Curie Intra European Fellowship within the 7th European Community Framework Programme.

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Correlative Use of Atom Probe Tomography and Electron Microscopy

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Many fundamental phenomena in materials science such as the segregation to defects, elemental partitioning, nucleation, deformation-driven phase decomposition, or spinodal decomposition need to be understood at the atomic scale, requiring mapping of local chemical composition and crystallography. This requires the development of suited characterization techniques. Atom probe tomography (APT) with its capability of detecting 3D elemental distributions with near atomic spatial resolution and a sensitivity in the range of 10 parts per million, which is independent of the atomic number [1] is currently the best high resolution tool for quantifying local chemical inhomogeneity. However, its spatial resolution is material dependent and often not accurate enough to capture crystallographic aspects such as defect type, grain orientations or phase crystallography. In these cases transmission electron microscopy (TEM) is better suited. But this technique lacks accuracy in quantifying chemical composition, especially in the case of light elements, high dilution and non-planar features. Thus, TEM and APT have complementary strengths and their correlated application to the same specimen provides joint chemical and structural insights to some of the main pending fundamental scientific questions in materials science.

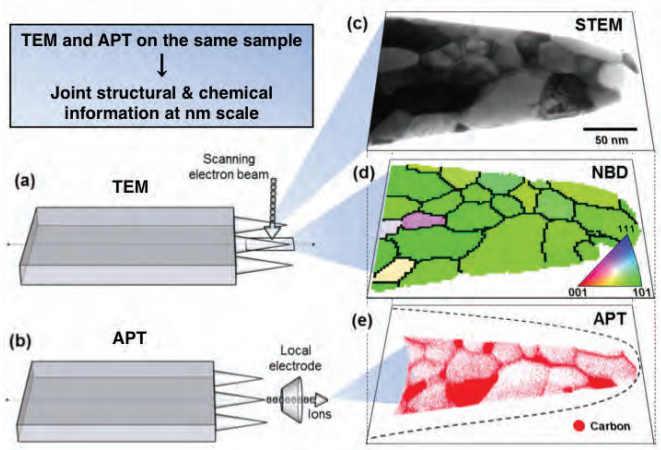

Fig. 1: *The correlative use of TEM (a) and APT (b) enables mapping both, structural and chemical information of the same sample at the nanometer scale [3].*

Over the past four years an experimental setup and corresponding know-how has been developed at MPIE rendering correlative TEM /APT experiments feasible and robust [2]. This work led so far to several high impact publications: for the first time nanobeam diffraction (NBD) orientation mapping was used on atom probe tips, thereby enabling the high throughput characterization of grain boundary segregation [3] (Fig. 1) as well as the crystallographic identification of phases [4]. Bright-Field STEM imaging enabled to prove the existence of linear complexions [5] and to map atomistic details associated with shear-induced mixing [6]. The spectrum of TEM/APT techniques is currently expanded to the correlative use of Dark-Field TEM and APT. Owing to the experimental efforts involved in correlative TEM/APT all scientific cases that do not require the spatial resolution of a TEM should be investigated by scanning electron microscopy (SEM). Therefore, SEM-based approaches to gather crystallographic information on atom probe samples have been developed [7,8]. Future plans involve the use of Electron Channeling Contrast Imaging under controlled geometric conditions (cECCI) [9] on atom probe samples that has the potential to speed up the site-specific sample preparation of crystal defects and their analysis. Intense collaborations with the department "structure and nanomechanics" are planned to combine latest high-resolution TEM instruments with a new atom probe with up to 80% detector efficiency.

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Unified Description of Interfaces between Electron-Conducting Solids and Ion-Conducting Liquids

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Solid-liquid interfaces are at the heart of many modern-day technologies such as water electrolysis and batteries, photo catalytic water splitting, electro catalysis or corrosion. A comprehensive understanding of the full reaction path of the complex electrochemical transformations inherent to any of these processes will aid a systematic development, improvement and optimization of any of them. This requires knowledge of the atomic and electronic structure of the interface and their evolution when environmental conditions change, as well as understanding of the reactivity (e.g. towards oxygen reduction, hydrogen evolution or metal dissolution) as a function of the atomic and electronic structure of a surface/interface. The heterogeneity of the interface and the complexities of the involved solid and liquid materials present a challenge to both experiment and theoretical modelling, requiring the development of experimental techniques which provide microscopic insight and of effective modelling techniques which account for the statistical averaging required to properly describe a liquid, allow reaching the equilibrium state and capture the essential properties of both the solid and the liquid. Hereby, the complementary use of experimental and theoretical approaches is of utmost importance and at the core of ongoing developments within the GO and the CM.

Our endeavour rests on several pillars. Optical experiments investigate the state of water at a solvated electrode/electrolyte interface by vibrational spectroscopy or use adsorption spectroscopy probing electronic transitions to study the defect structure in thin oxide films. Combining experiments with different depth-dependence allows to study electrodes immersed in both thin water films and bulk electrolyte, but also look into intermediate steps by probing solvation using the Surface Force Apparatus (SFA) (few nm), probing solvation in nano-channels (few 10 nm) or probing solvation by angular dependent internal reflection infrared spectroscopy (few 100 nm). Complementary high-resolution force probe and imaging experiments focus onto electric double layer structures. The unique advancement of single molecule desorption studies allow direct measurements of interaction free energies of tethered functional groups with model surfaces [1], of metal interfaces [2] and of arbitrary functionalities. These experiments will be extended to surfaces under varying electrochemical and environmental (e.g. ΔpH and ΔE) conditions enabling experimental measurement of the interaction free energy of molecules with hydrated electrochemically active interfaces. Several of these experiments provide information accessible by first principles based calculations, which provide the opportunity to benchmark theoretical modelling approaches. Thus, theoretical efforts focus on methodological developments (see p. 161 and [3]) aiming at a realistic description of processes at the solid/liquid interface, but also benchmark individual constituents of the solid/liquid interface or the interface itself, which will provide a firm basis to optimisation of modelling approaches. One example is the effort to acquire accurate ion hydration energies (see p. 75), another, the calculation of spectra for aqueous systems (see p. 29) to probe, e.g., the well characterised phase transition between the pristine and the H covered water/Ge interface. The proper description of electric fields within the constraints given by the periodic boundary conditions and cell-size restrictions of density-functional theory codes will be addressed in the near future.

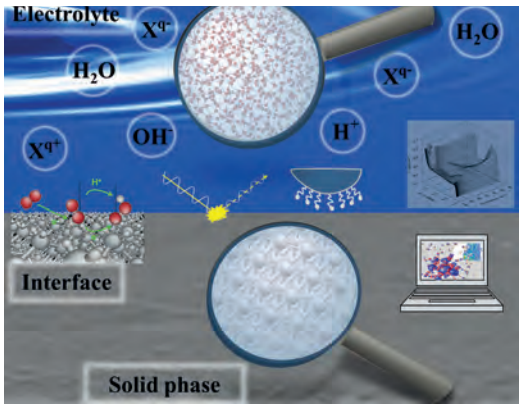

Fig. 1: *Schematic representation of the solid/liquid interface. Insets show atomistic details of the constituent condensed phases and interface processes or point at some of the experimental techniques and computational approaches used in our studies.*

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Electrochemical Scanning Flow Cell for Combinatorial Reaction Analysis

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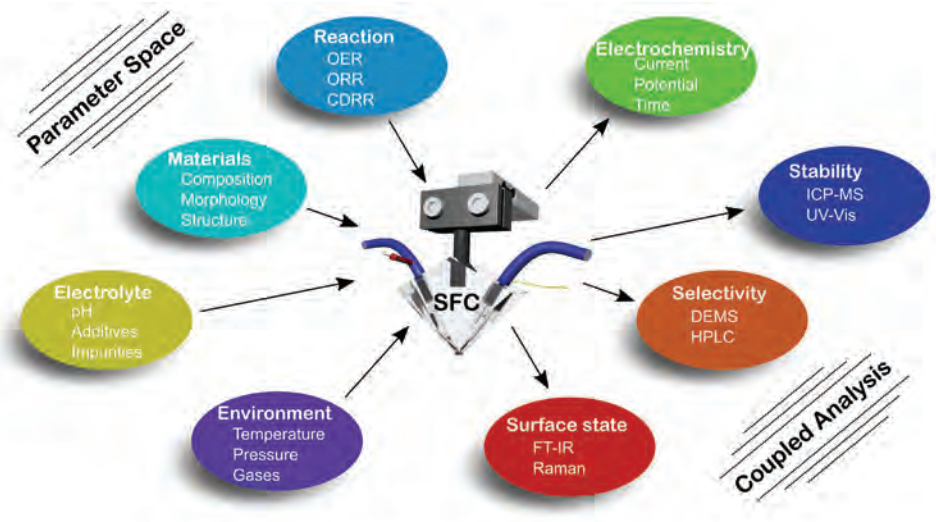

Fig. 1: *Concept of the combinatorial reaction analysis by SFC coupled techniques.*

In the 21st century the fraction of renewable energy in the overall energy mix will steadily grow. This energy will have to be efficiently distributed, converted, and stored to be utilized to full extent, which can be done with modern electrochemical technologies. In this regard, electrochemistry can be portrayed as a "bridge" between electrical and chemical energy. In reality, to improve the efficiency of energy conversion and thus serve the needs satisfactorily, this bridge requires a support – electrocatalysts. The latter have to be active, stable, abundant, environmentally friendly, and cheap. Understanding the fundamental mechanism and identification of the optimum electrocatalyst for each individual reaction is the main challenge of modern electrochemistry. The most promising tools in this quest are high-throughput experimental approaches, as only such techniques are capable to deal with the complex parameter space that influence electrocatalysis, and can deliver the data required to derive an understanding of the processes involved. The unique electrochemical scanning flow cell (SFC), a workhorse developed in the "Electrocatalysis" group, is a combinatorial approach that can cope with all the requirements and that has been successfully applied for various reaction analyses (Fig. 1) [1].

A typical example that has become increasingly important recently is the oxygen evolution reaction (OER) [2]. Finding optimal material properties and reaction conditions to catalyze the OER is done by fast scanning of material libraries, e.g. thin film gradient samples. The catalyst efficiency is then estimated directly from electrochemical analysis. Stability information, which is most crucial in the case of the OER, is provided by time- and potential-resolved inductively coupled mass spectrometry (ICP-MS) analysis. As soon as an efficient and stable catalyst is identified, this strategy changes to the investigation of electrolyte properties and operating conditions for the parameter optimization. The obtained information is utilized for the synthesis of high surface area catalyst materials, which are also studied initially with the SFC, and finally are employed in the development of more efficient electrolyzers. To name only a few, other important reactions addressed by the SFC are the oxygen reduction reaction (ORR) for fuel cells, carbon dioxide reduction reaction (CDRR), but also classical corrosion processes [3, 4].

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Scanning Kelvin Probe Techniques

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The recent development at the MPIE to use Kelvin Probe techniques such as Scanning Kelvin Probe and Scanning Kelvin Probe Force Microscopy for spatially resolved high sensitivity measurement of hydrogen has been a major break-through for our work on hydrogen in materials [1]. One big task at the MPIE is therefore to further develop Kelvin probe techniques for hydrogen mapping (see p.39).This success also demonstrated that this contact-free technique for measuring electrode potentials on surfaces and at buried interfaces may hold also further possibilities for exploitation.

One idea is to use the ability to detect hydrogen at very high sensitivity for detecting corrosion sites through the metal, i.e. for instance to measure internal corrosion at the outside of a pipeline or a tank, i.e. through the metal wall. This should allow detecting corrosive attack already before measurable loss of metal. However, for such application a more robust Kelvin Probe device has to be developed that can be used in the field. The development of such a Kelvin probe is a project carried out together with Christian Michelson Research (CMR) institute in Bergen, Norway. From the scientific point of view a number of very interesting issues have to be investigated, such as the detection of hydrogen also through organic coatings and how to deal with trapped charges in coatings.

Another method which is currently being developed is to use the Kelvin probe technique for measuring electrochemical reaction rates at buried interfaces. Up to now this was not possible, although this would be of great importance. For instance, the electrochemical stability of the buried metal-organic coating interface of painted metal is crucially governed by how effectively the oxygen reduction reaction at the interface is inhibited. As this interface is not directly accessible for study by conventional electrochemical techniques, a new non-destructive method has to be developed. For assessing the oxygen reduction rate under buried interfaces we chose to measure the potential resulting from equilibrium between oxygen reduction and hydrogen oxidation. The hydrogen is supplied from the backside of the sample where the hydrogen uptake current is also monitored. One of the crucial points here is to ensure that all the hydrogen produced at the hydrogen entry side is really entering the metal. If so, by measuring the potential at the coated exit side a full I(U)-curve can be thus constructed. Thus oxygen reduction rates at buried interfaces now have become accessible [2].

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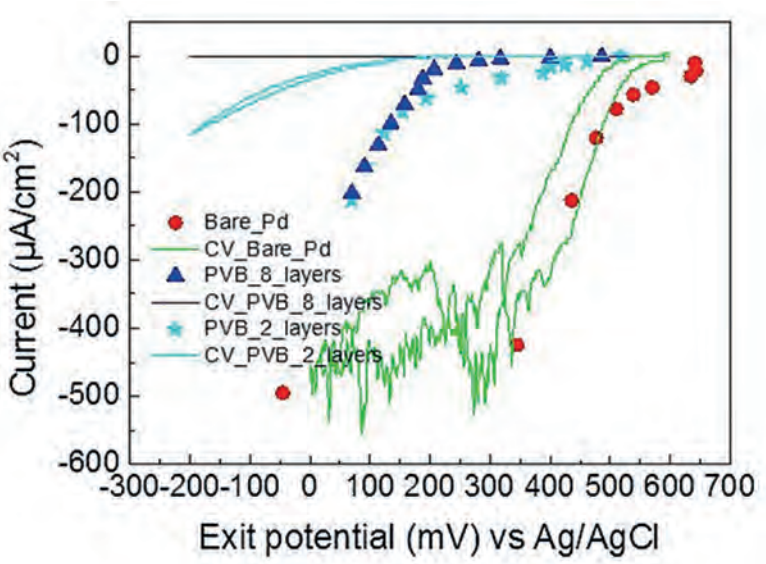

Fig. 1: *Cyclovoltammograms (CV) measured on a Pd surface in acidic solution of pH1, bare surface (green solid line), one time PVB coated surface (light blue line), twice coated surface (dark blue line). The symbols show the results obtained by the new methodology. Interesting: the oxygen reduction rate measured with the new technique shows the same rates for the once and twice coated surface. This is to be expected as the interface is the same. The corresponding CVs are different, as these just measure the pin holes and cannot access the buried interface.*

Hydrogen Mapping

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From novel high strength steel grades via Ni-based superalloys to modern aluminum alloys, hydrogen related degradation of materials plays an increasingly important role in current materials development. This is not only because they are very susceptible to hydrogen embrittlement, but also because technical application ventures into increasingly aggressive environments, as it is the case e.g. for the oil industry where sour gas environments can lead to very high hydrogen activities. Therefore, the topic is and will remain of crucial importance and is addressed within various publically and industrially funded projects at the MPIE.

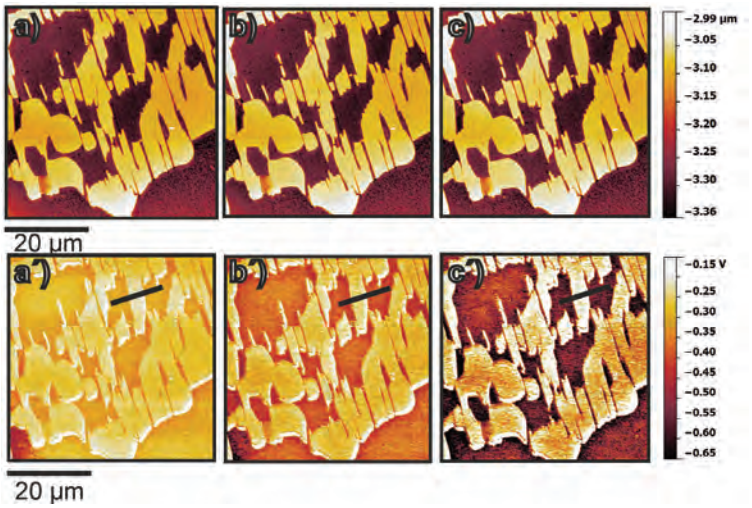

Fig. 1: *Results of an SKPFM measurement on a Ni-22wt-% (15at.-%) Nb alloy charged with H and measured 20 h, 50 h and 100 h afterwards. Upper row: topography, revealing that after etching the Ni3Nb intermetallic phase stands out higher than the Ni matrix. Bottom row: potential difference maps, providing a higher H effusion from the matrix than from the intermetallic phase as the contrast increases with time. Lower potentials correspond to higher H concentration in the Pd layer.*

Such projects are needed, since for an in-depth understanding of the degradation mechanisms a detailed characterization and simulation of the materials with respect to their microstructure and of the hydrogen distribution therein are important. For the latter, a number of different experimental techniques are already available at the MPIE, such as the silver decoration technique, microprint technique, tritium autoradiography and time-of-flight secondary ion mass spectroscopy (ToF-SIMS). Additionally, a novel approach based on the Kelvin Probe technique for hydrogen mapping has recently been developed in the GO [1, 2]. Its key strength is to add to a pure H mapping the important information on binding energies at different sites by directly measuring the hydrogen release from the investigated material into an ultra-thin palladium detection layer with high local resolution (Fig.1). Hence, a time dependent contrast between the different phases is measured. Up to now the AFM (Atomic Force Microscopy) based Kelvin Probe technique, the so called Scanning Kelvin Probe Force Microscopy (SKPFM), cannot be reliably calibrated and thus only relative hydrogen release rates of different phases and features such as grain boundaries can be obtained.

It is therefore decisive to combine the achieved insights with *ab initio* based simulations of the hydrogen solubility within the different phases as performed by the CM. Using high-throughput concepts, this research considers besides microstructure features also the impact of all alloying elements in the investigated materials.

On the experimental front, SKPFM is currently combined with standard SKP (Scanning Kelvin Probe), which allows the full quantitative measurement of release rates into the palladium layer, in order to obtain highly resolved quantitative information.

In order to obtain direct information about the local concentration of hydrogen, techniques, such as e.g. atom probe tomography or ToF-SIMS are used. As these are surface sensitive techniques most hydrogen that was in the sample during hydrogen charging, will have left the relevant region when the measurement starts, i.e. the measurement will be affected by the effusion rate from the material, which in turn is measured by the Kelvin Probe techniques. It is the aim of this long-term method development to develop routines for a combination of these experimental and theoretical techniques, in order to achieve a detailed characterization of hydrogen inside complex materials.

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Grain Boundaries: Interfaces of Outmost Importance in Materials

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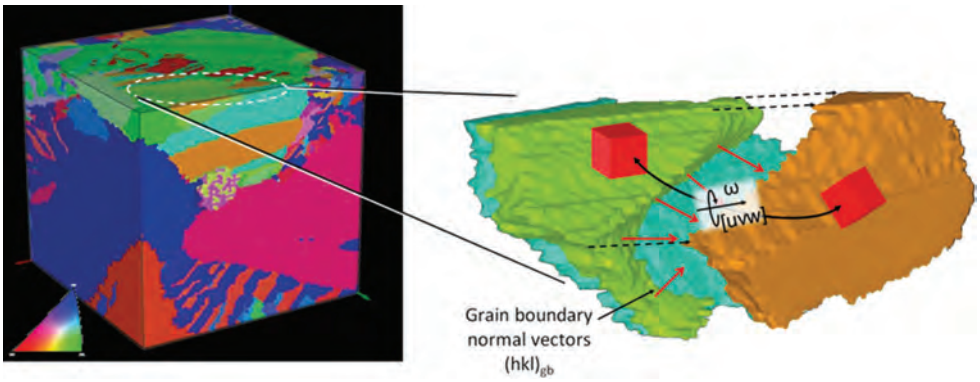

Fig. 1: *Three dimensional reconstruction of a polycrystalline microstructure analyzed by 3D-EBSD.*

Most structural and functional materials are polycrystalline with grain size and grain boundaries impacting their mechanical behaviour (strength, ductility) [1], corrosion resistance and, e.g., opto-electronic properties. Thus, grain boundaries are a central theme of all departments connecting several research groups at the MPIE.

The bare number of unknowns and variables in one grain-boundary exemplifies the degree of complexity in a nominally simple interface. Crystallographically, the grain-boundary can be described by only five variables: three parameters describing the misorientation in between the two adjacent grains; and two parameters describing the grain-boundary plane. But if it comes to mesoscopic dimensions, it can be noted that most grain-boundaries are not straight, they are curved. A trend which is continuous if zooming into the atomic scale, where atomic positions in the vicinity of the boundary are significantly off their predicted crystalline positions. In terms of pure metals this is the maximum complexity one can possibly encounter. But engineering materials involve another dimension: Their chemical composition across the boundary is far from being homogenous – a fact which opens new routes for tailoring material´s properties at all length scales.

During the past years several attempts have been undertaken to get closer to a broad understanding of the role of grain boundaries. Besides advanced microstructural characterization techniques (e.g. TEM (Transmission Electron Microscopy) including High Resolution-TEM, 3D-APT (Atom Probe Tomography, 3D-EBSD (Electron Backscatter Diffraction), µLaue, *in situ* micromechanics) also simulation techniques bridging across all relevant length scales – from atomistic to macroscopic – had severely been applied to understand grain boundaries.

The MA combines FIB (Focussed Ion Beam)/ SEM-EBSD tomography with other tools like cathodoluminescence or local mechanical testing [2] to study the crystallography of boundaries at the mesoscopic level and to obtain, at the same time, information on the properties of these boundaries. APT gives important information on the chemistry of boundaries [3] required to understand, for example, the strength of a material or the formation of new phases at boundaries. Within the SN the work focusses on two questions: (i) can we quantify models for dislocation slip transfer (e.g. [4]) and (ii) what is the impact of dislocation source size distributions as one origin of sample size effects on the dislocation transfer mechanisms. The CM investigates the migration kinetics of grain boundaries in Al using atomistic simulations [5], revealing the fundamental mechanisms involved in the motion of grain boundaries at experimental time/length scales. The cover-picture of this report highlights one of our important findings on the atomistic details of grain boundary migration.

The research activities in the different departments unraveling the important role of grain boundaries are increasingly bundled with new insights by applying complementary experimental techniques and corresponding simulations.

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Electron Channelling Contrast Imaging (ECCI) for Direct Observation of Lattice Defects in Bulk Samples

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Electron channelling contrast imaging (ECCI) is an electron diffraction-based technique for direct observation of individual crystal lattice defects, like dislocations, stacking faults or nano twins, on bulk specimens using the scanning electron microscope (SEM). Although the technique is long time known, it has recently regained interest [1][2], mainly caused by the technological advances in SEM design. In particular, observation of ECC requires an electron beam with very small convergence, small focus point, high beam current and a large but quick detector for backscattered electrons. These contradicting requirements are nowadays satisfied by dedicated SEMs allowing to obtain images of lattice defects with a resolution of better than 10 nm. Though the contrast is less than that in scanning transmission electron microscope (STEM) images, ECCI has the large advantage to give images from bulk samples, looking up to about 100 nm below the surface. An application example for this powerful technique is our recent study on dislocation evolution in a quasi-single crystal superalloy during creep. The observations were done on full cross sections of a test sample in areas of different total stress and strain. As a result it was found that creep dislocations do not only originate from the small-angle interdendritic boundaries, as it was long time assumed [3], but a significant contribution is made by dislocations nucleating in the interior of the dendrites from individual dislocations being scattered therein [4]. The figure below shows ECCI of dislocations nucleated in the interior of the grain (c) and those nucleated at interdendritic boundaries (d), under a load of approximately 330 MPa. The former ones are indeed much denser. This density difference could also be confirmed by discrete dislocation dynamics simulations carried out for both scenarios.

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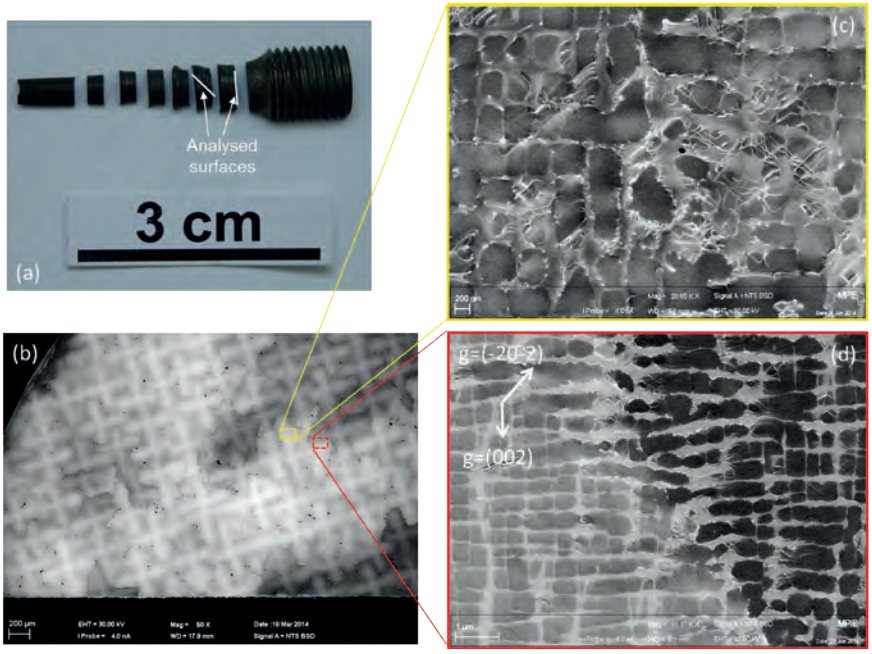

Fig. 1: *Dislocation observation in a crept single crystal superalloy test specimen (950° C, 450 MPa), using ECCI. (a) the macroscopic sample, (b) overview on the dendrite structure, (c) dislocations in the dendrite interior, (d) dislocations at a dendrite interface.*

New insights into Microstructures by Application of Advanced High-Resolution SEM-Based Diffraction Techniques

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Electron backscatter diffraction (EBSD) is a well-established diffraction technique in scanning electron microscopy. A particular strength of 2D and 3D EBSD-based orientation microscopy is its quantitative nature. In contrast to other microscopy techniques it does not, originally, deliver images but numbers for every scan data point from which images and many other information can be calculated. One example for such a value is the density of geometrically necessary dislocations (GND) that can be calculated as the tensor curl of the 3D orientation field [1]. In contrast, statistically stored dislocations (SSD) are not directly accessible from conventional EBSD although the density of SSDs is as important for evaluation of the total stored dislocation density of a material as that of GNDs. To overcome this deficit a new powerful EBSD analysis method is currently being developed which is Kikuchi band profile analysis based on the newly developed Kikuchi bandlet method [2]. The method functions similar to x-ray peak profile analysis but with the serious complication that Kikuchi lines are created by dynamic rather than kinematic diffraction. Quantification of dislocation densities from these peak profiles is a challenge which we currently approach by a calibration method using dynamic diffraction-based simulation of EBSD patterns from crystals with defects. A first result of peak profile analysis is displayed in the figure: A peak profile sharpness parameter extracted for various bands of a diffraction pattern undergoes significant changes over a deformed single crystal. This may indicate that different slip systems are active in different areas of the sample, leading to different blurring of different Kikuchi bands in the EBSD patterns. The Kikuchi bandlet method has further attractive applications like improved orientation accuracy, and, potentially, absolute elastic strain determination from individual EBSD patterns [3].

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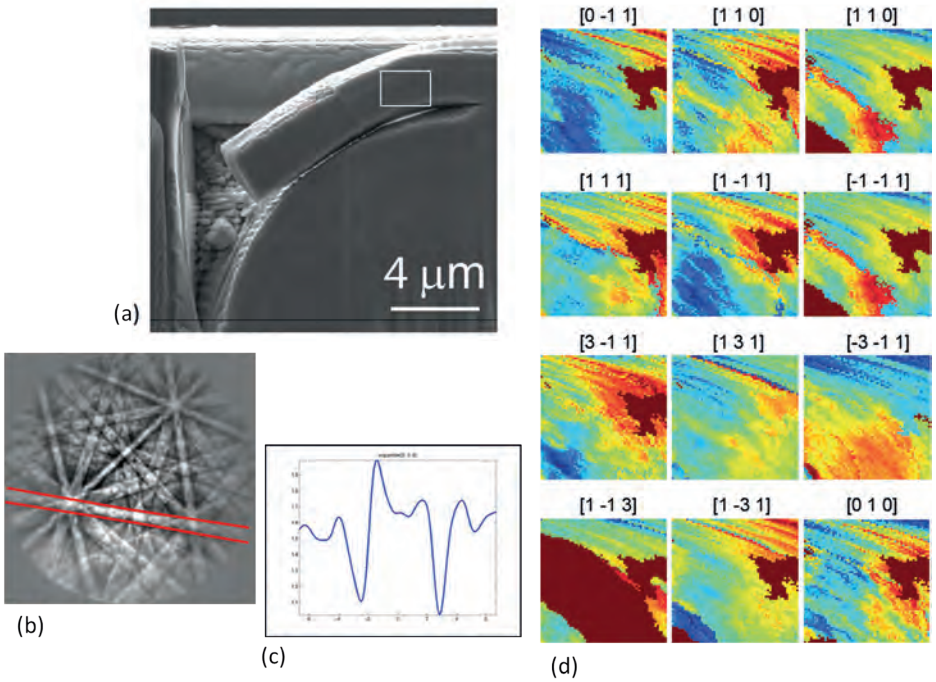

Fig. 1: *Plastic strain characterization in a bent microcantilever (a), using the Kikuchi bandlet technique (b) to obtain band profiles of different Kikuchi bands (c). Band profile sharpness maps for different Kikuchi bands are displayed in (d).*

Bright Light on Plasticity: *In situ* µLaue Diffraction

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Interlinking the mechanical response with the underlying and evolving crystallography and microstructure is the key to define material models and to formulate mechanism-based material laws. It requires dedicated *in situ* techniques being able to observe the collective behaviour of a limited number of defects (e.g. dislocations). Within the last years capabilities to deform micron-sized objects in highly brilliant, focused white x-ray light in Laue geometry (*in situ* µLaue) had been developed and implemented at the French beamline CRG-IF at the European Synchrotron Radiation Facility [1].

µLaue diffraction is well able to quantify crystallographic phase(s), orientation(s), deviatoric strains and density of geometrically necessary dislocations (GNDs). Our experiments are typically performed with a 500 nm sized white x-ray beam with a spectral range of 5-22 keV. A self-made loading rig was developed at the MPIE and today allows for a displacement-controlled deformation of micron-sized test specimens in compression, tension, bending and fatigue. Typical force and displacement resolution reach micro-Newton and nano-metres. The device operates in full displacement-controlled mode with strain rates from 10^{-4} s^{-1} up to 10^{-1} s^{-1}.

The application of the technique covers several important research topics across the MPIE, like size effects in materials in uniaxial [2] and cyclic loading [3], the dislocation grain-boundary interaction [4] as well as deformation behaviour of complex microstructures [5,6], investigated together with the department of Microstructure Physics and Alloy Design. Thus, µLaue diffraction is one of the corner stones of the SN and micromechanics group.

In future, the main focus is to put on the improvement of data interpretation (“3D-EBSD informed Laue analysis”) as well as implementation of non-ambient temperatures and media in the straining device.

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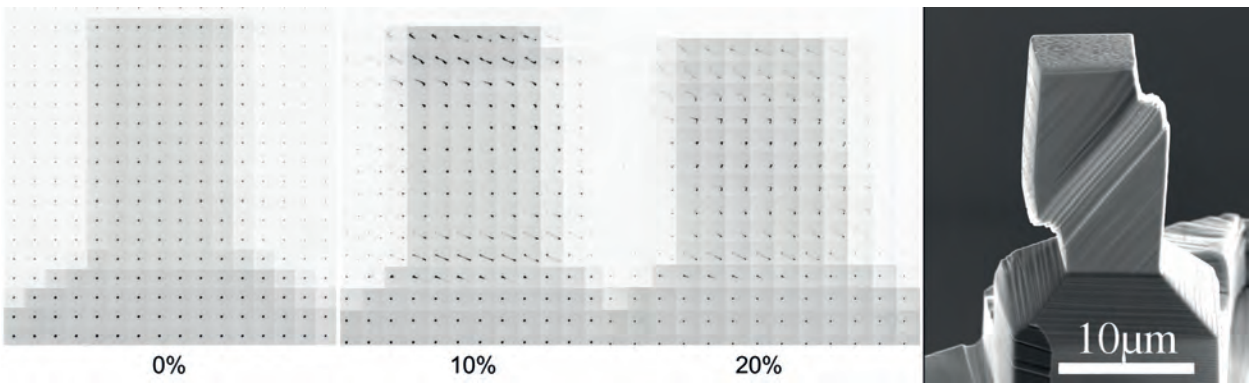

Fig. 1: *µLaue composite images of a copper micro pillar. The x-ray beam is scanned across the entire 7x7x21 µm³ sized samples and the representative (111) reflection at various locations is plotted. At 0% engineering strain (left) the spots are all circular, indicating the lack of stored GNDs. During stepwise straining to 10% and 20% GNDs are stored in the top and bottom part to accommodate for experimental constraints. The scanning electron microscope(SEM) image to the right shows that the deformation is confined to only few slip steps, documenting that the two methods are complementary: µLaue probes stored dislocations, SEM slip step analysis not.*

Innovative Material Synthesis

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Within the group Combinatorial Metallurgy and Processing about 500 metallic materials are synthesised every year for both internal projects – with all departments – as well as external cooperations with scientific and industrial partners. This represents the basis to investigate micro- and nano-structural phenomena, validate simulations and study complex transient phenomena such as non-equlibrium phase transformations and interfacial reactions. Accordingly a wide range of experiments are performed, from highly controlled syntheses of single- or oligo-crystaline materials, to binary model alloys, as well as modified industrial materials. The corresponding solidification kinetics can be controlled from quasi-equilibrium conditions up to extremely rapid cooling required e.g. for amorphous metallic glasses.

The spectrum of the advanced structural materials ranges from novel lightweight titanium- or magnesium alloys, to intermetallic materials and high entropy alloys, which is made possible by the high level of qualification and experience of the technical personnel. The main expertise, however, lies on the synthesis and processing of innovative iron based materials, such as lightweight-construction steels [1]. Currently, the main focus lies on *in-situ* metal-matrix-composite steels with an improved stiffness / density ratio [2], also termed high modulus steels (HMS). We recently demonstrated how particles such as titanium diboride can be refined down to the nanometric range with liquid metallurgy synthesis production techniques, thus overcoming the inherent conflict between physical and mechanical properties (Fig. 1).

The design of this multitude of novel materials goes hand in hand with the development of innovative synthesis and processing routes with differing scopes [3], all embedded into developments stretching over a long term and in strong interaction with other groups and departments. Innovative methods for the accelerated synthesis, processing and testing of bulk metallic structural materials are developed and deployed, thus reducing the time between an alloy design idea and the final evaluation of the materials´ mechanical and microstructural properties from several weeks or even months down to hours [4].

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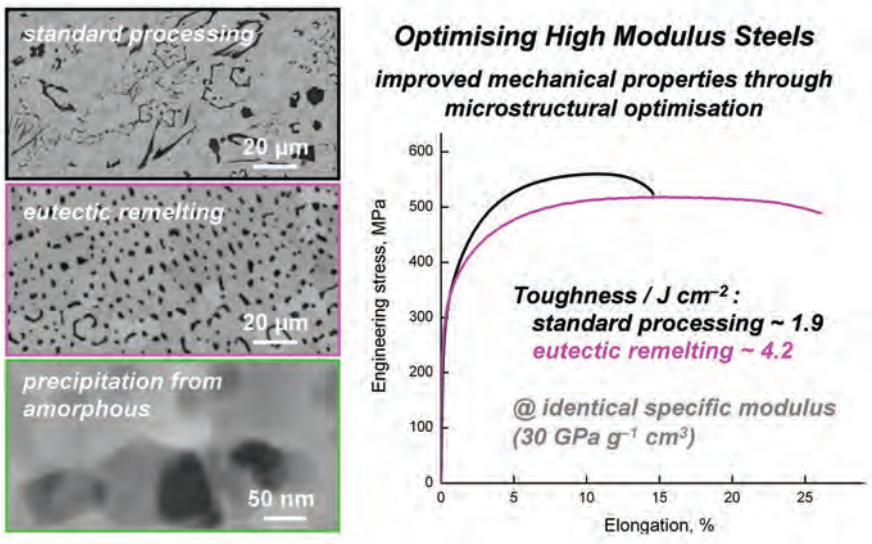

Fig. 1: *Innovative material synthesis, here exemplified on the optimisation of stiff and lightweight high modulus steels: improved mechanical performance (right) through refinement of shape, size and dispersion of TiB2 particles in Fe matrices (left, dark particles) by controlled solidification kinetics.*

The Düsseldorf Advanced Material Simulation Kit: DAMASK

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Crystal plasticity modelling has matured into a cornerstone of computational materials science [1]. Devel-oping this field from its original mean-field homogenization approach in conjunction with viscoplastic constitutive hardening rules into an advanced multiphysics continuum field solution strategy requires a long term initiative. Roter's "Theory and Simulation" group is working in this field since 2000. Starting originally from Kalidindi's numerical crystal plasticity integration scheme [2] user subroutines for the commercial FEM (Finite-Element-Method) packages Abaqus and MSC.Marc were developed. The scientific focus of the group was, however, the development of advanced constitutive models based on dislocation densities as internal state variables, which are capable of providing microstructure based predictions [3]. As simulations of different material classes and on different length scales necessitate the use of constitutive descriptions of varying degree of sophistication, it soon turned out that the numerical implementation was not flexible enough to incorporate different constitutive models. Therefore, within the project "Computational Modelling of Polycrystals" (CMC^n, the first joined MPG-FhG project ever, established in 2006) the development of a flexible framework, for crystal plasticity simulations on all scales from the single crystal up to the engineering component, was initiated. The new code is strictly modularized to allow easy incorporation of additional models on all length scales. In this way, two different homogenization schemes and seven different constitutive models for plasticity, including a non-local one treating dislocation fluxes [4, 5], have been incorporated into the code package. The ability to use different constitutive models within a single simulation is a unique feature of the code. In 2010, in collaboration with Prof. R. Lebensohn (Los Alamos National Laboratory, Humboldt awardee at MPIE at that time), a spectral method based boundary value problem solver was added to complement the commercial FEM solvers. In 2011, it was decided to release the code, by now called DAMASK, as free software to the public domain. For that purpose, a website (damask.mpie.de) was launched in September 2011. The science community very well received the idea of a free crystal plasticity code. At least 15 groups, including universities like the University of California, research facilities like the Los Alamos National Laboratory as well as companies like Tata Steel (IJmuiden), today use DAMASK worldwide (as it can be freely downloaded we do not know the real number). These groups contribute to the further code development as well as adding new features to DAMASK including new/modified constitutive models [6]. Currently, DAMASK is extended towards a multi-field solver. This will allow treating coupled problems, e.g. thermo-mechanical-chemical, in a fully consistent way.

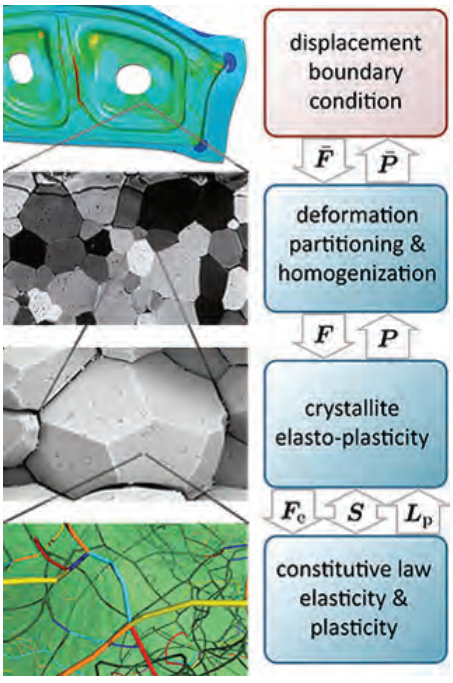

Fig. 1: *Hierarchy of scales as treated in DAMASK.*

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Ab initio Thermodynamics for Materials Design

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A central aim of the CM is the development and application of techniques that allow for an efficient and accurate computation of thermodynamic properties at finite temperatures from *ab initio*. A severe challenge in such computations is that free energies of the various phases are almost degenerate, often requiring to resolve energetic changes below 1 meV/atom. The theoretical formalisms therefore need to accurately capture all relevant entropic contributions due to electronic, vibrational or magnetic excitations, as well as their coupling such as phonon-phonon, magnon-phonon interactions or spin-quantization.

Over the past ten years the CM has combined accurate first principles calculations with advanced statistical sampling methods allowing now to address these issues and to determine free energies and derived thermodynamic quantities that often rival available experimental data. Our efforts recently allowed us to develop and implement a wide range of optimized methods for various tasks such as, e.g.:

- the random-phase-approximation upsampled thermodynamic integration using Langevin dynamics (RPA UP-TILD) to include electronic correlation effects in finite temperature calculations [1],
- the local anharmonic (LA) approximation to highly efficiently capture anharmonicity of solids with a few T = 0 K calculations only [2],
- the two-stage upsampled thermodynamic integration using Langevin dynamics (TU-TILD) method to accelerate anharmonic simulations of arbitrary structures and phases [3],
- the local Grüneisen theory (LGT) to accurately capture the observed non-Arrhenius behaviour for point defects [4],
- the extended spin space averaging (SSA) method to describe magnetic disorder [5].

Besides providing an efficient and accurate sampling of the phase space, these approaches give also a direct insight into the fundamental physical mechanisms responsible for the finite temperature energetics. A few selected applications are exemplified in the figures.

Long term developments in this field will be focused on the extension of these methods to alloys, extended defects, and liquids, all of which are decisive for the understanding and design of structural and functional materials.

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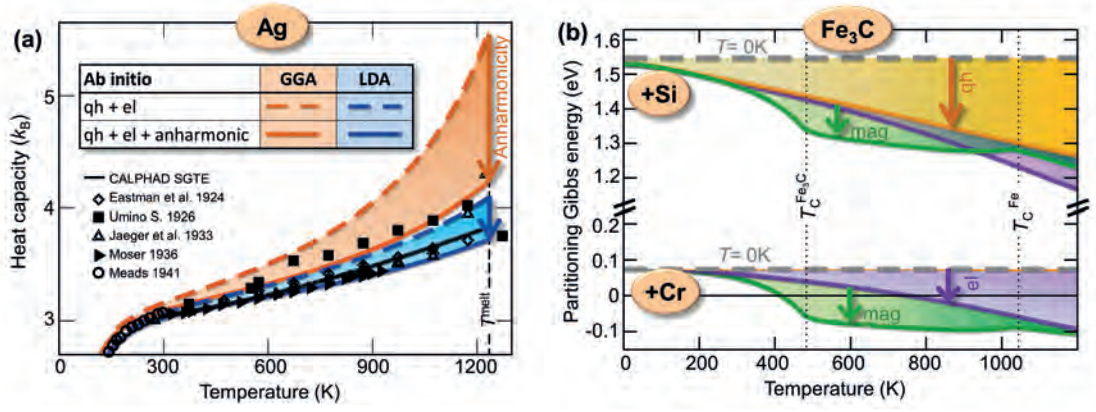

Fig. 1: *Recent examples for ab initio thermodynamics: (a) Impact of anharmonic phonon-phonon interactions (shaded region) on the heat capacity of Ag [1]. (b) Partitioning Gibbs energies between ferritic iron and cementite for Si and Cr. The influence of vibrations (qh), electrons (el), and magnetic (mag) excitations is shown and the Curie temperatures of cementite and ferrite are marked with the dotted lines [6].*

Large-scaled and Networking Projects

The International Max Planck Research School SurMat – Interface Controlled Materials for Energy Conversion (IMPRS-SurMat)

Previously: International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS-SurMat)

E. Gattermann, A. Erbe

The IMPRS-SurMat is a structured, three-year doctoral programme coordinated at the Max-Planck-Institut für Eisenforschung since 2004. During the second running period (till December 2015) the focus was broadly on materials interfaces. Research groups from the Ruhr-Universität Bochum, the Interdisciplinary Centre for Advanced Materials, the Max-Planck-Institut für Kohlenforschung and the Max-Planck-Institut für Eisenforschung brought their various competences together, and they lead interdisciplinary projects to outstanding results. The close link between experimental and computational science enhanced this effect.

In April 2014, the IMPRS-SurMat was very successfully evaluated. The external reviewers were impressed by the excellent scientific output by the IMPRS-SurMat students and by the future concept. Further, all partners assured a substantial own financial contribution. The new concept, briefly outlined below, also convinced the state of North Rhine-Westphalia to contribute financially to the new school. All reviewers recommended therefore the continuation of the school. The responsible committee of the Max Planck Society followed this recommendation and the IMPRS-SurMat got extended for its third period that will last from 2016 till 2021. Consequently, in January 2016, the third running period of the International Max Planck Research School SurMat begins. This prolongation will bring some major changes.

During the last years, new key aspects came into the focus of all partners. Many groups work now on topics important for the development and understanding of materials for energy conversion. Two further institutes of the region are dealing with these aspects: the Max-Planck-Institut for Chemical Energy Conversion and the University Duisburg-Essen. Groups from both institutions could be won to join the IMPRS-SurMat and will officially join the programme with the beginning of the new period in January 2016. With this step, the main players of the Rhine-Ruhr region in the field of materials interfaces are coming together in the IMPRS-SurMat.

The scientific topic “Interface Controlled Materials for Energy Conversion” shall combine the strengths of the partners and focus on four topics:

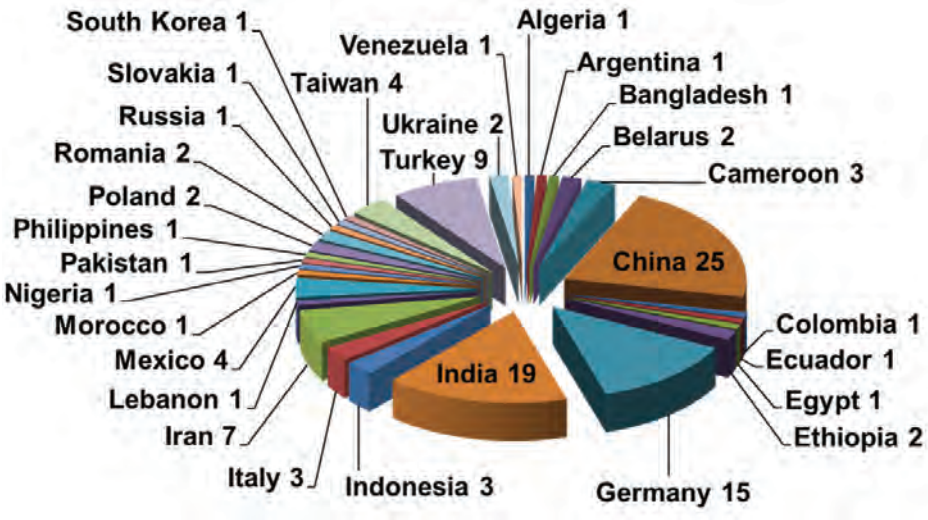

Fig. 1: *Origin of IMPRS-SurMat students by countries.*

• Microstructure and physics of defects

• Hydrogen and oxygen technology

• Materials for future energy systems

• Degradation mechanisms and life extension of materials

In April 2015, a kick-off workshop for the new period took place at the MPIE. The professors and departmental directors of the current and the new partner institutes presented their research fields and how they plan to contribute to IMPRS-SurMat projects. The IMPRS-SurMat students presented the current research work in a poster session. This fruitful workshop lead to the start of several new projects already in 2015.

For the doctoral students, the programme continues to offer a well-balanced curriculum and ensures the best available supervision. The programme is conducted entirely in English and the doctoral degree (Dr. rer. nat or Dr. Ing.) is conferred by one of the partner universities. The school offers funding for three years, but is also open to students funded from outside as long as all required criteria are met.

The core curriculum remains to be delivered over years one and two. It is structured as a series of four two-week classes each term (winter/summer) that explore various aspects of modern materials and interface science. In addition soft skill trainings, such as presentation skills, scientific writing, project management, and career development events – the latter in the form of career talks given by industry contributors - are taking place regularly.

Each project is supervised by at least two scientists from different departments and institutes. Thus, the interdisciplinarity is guaranteed. Once per year, the doctoral students send a short report about the progress of their work to the programme coordinator. Subsequently, Thesis Advisory Committee (TAC) meetings take place to discuss the results and plan the next working steps. Previously, TAC meetings took place only after the second year.

From 2004 on, 118 students from 28 different countries joined the IMPRS-SurMat. Most of them came from Asia (China, India, Iran), but there are also students from Europe, Africa, Middle and South America. To get admitted the students have to apply online in one of the two application rounds taking place per year. The application process has continuously evolved into an efficient selection procedure. All shortlisted applicants are invited for personal interviews. After a descent of admissions in 2014 because of the evaluation and planning of the new period, already 15 new students were admitted in 2015 to start with the new concept and to integrate the new partners.

Since 2004, 65 students have successfully finished their doctorate within the IMPRS-SurMat (23 students from 2013 till 2015), the duration of the doctoral work is in the most cases between 3 and 4 years. The scientific output is genuinely high. Besides more than 170 poster and oral presentations on conferences, 287 journal articles have been published.

With the new partners and the new concepts, we are looking forward to a successful third running period of the IMPRS-SurMat.

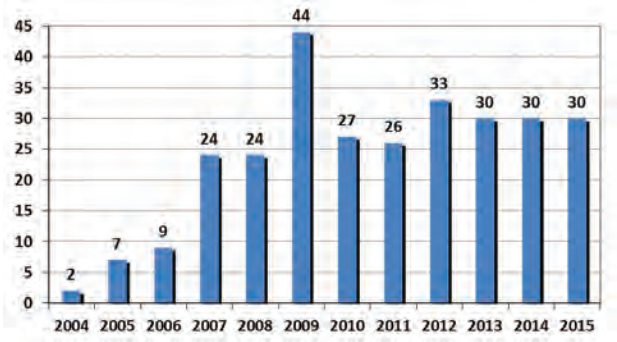

Fig. 2: *Number of publications by IMPRS-SurMat students in peer reviewed journals.*

Fig. 3: *IMPRS-SurMat community at the annual retreat in 2014.*

Gas Turbines of Tomorrow: From Atom to Turbine Blade – Scientific Foundations for a New Generation of Single-Crystalline Superalloys SFB/TR 103

I. Povstugar, Z. Peng, R. Li, A. Kostka, P. Choi, D. Raabe

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Ni-base superalloys are the key engineering materials for high-temperature applications, such as aircraft engines or land-based turbines for electrical power generation. The collaborative research centre SFB/Transregio 103, devoted to comprehensive understanding of superalloy structure and properties, was established in 2012 at the Ruhr-Universität Bochum and the Friedrich Alexander University of Erlangen-Nürnberg. The MPIE participates at the SFB/Transregio 103, performing 3D characterization of alloy chemistry by means of atom probe tomography (APT). This method provides essential information on elemental partitioning and segregation within the microstructure

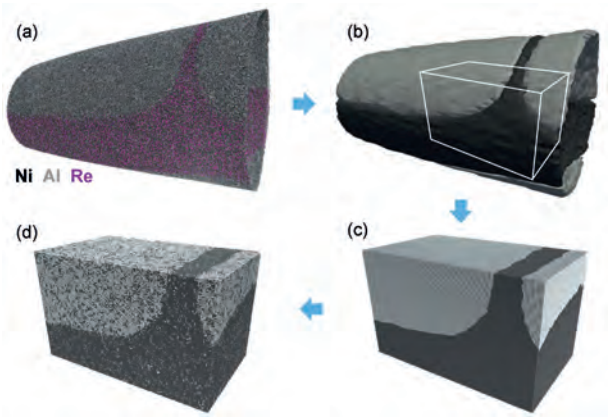

Fig. 1: Generation of atomistic simulation samples from APT data. (a) Reconstructed APT specimen (only Ni, Al and Re shown). (b)-(d) Use of reconstructed iso-density surfaces of Al (gray) and Re (black) for developing a non-stoichiometric APT-informed atomistic sample with realistic atomic configurations.

of Ni-base and novel class of Co-base alloys, on elemental redistribution under creep deformation and formation of deleterious topologically close-packed (TCP) phases.

Experimental APT data for an industrial CMSX-4 alloy were used for generating a realistic sample for atomistic simulations (Fig. 1) in order to study the interaction between γ-channel dislocations and γ' precipitates [2]. It was shown that the precipitate morphology, in particular its local curvature, and the local chemical composition significantly alter both the misfit dislocation network at the precipitate interface and the core structure of the misfit dislocations. APT-informed simulated tensile tests reveal the atomic scale details of many experimentally observed dislocation-precipitate interaction mechanisms, which cannot be reproduced by idealized simulation setups with planar interfaces.

Precipitation of TCP phases, which have a detrimental effect on creep lifetime of alloys, was another important topic. Ru is known to significantly slow down TCP phase formation, but the exact mechanisms of the Ru effect on elemental partitioning and TCP phase precipitation have been under debate for a long time. For a series of complex Ni-base superalloys, Ru was shown to partition equally to γ and σ (TCP) phases and significantly reduce TCP precipitation. However, Ru did not lead to notable changes in partitioning of other elements or to their segregation at phase boundaries [3, 4]. The earlier proposed hypothesis of 'reverse partitioning' (redistribution of Re content from γ to γ' caused by Ru) was disproved and an alternative mechanism proposed, which involves an increase in lattice misfit between the σ-phase and the parent γ-phase in the presence of Ru and resulting in an increase in nucleation barrier.

Besides Ni-base alloys, a new class of γ'-strengthened Co-base alloys was investigated with a focus on the influence of alloying elements on the microstructure and mechanical properties. The elemental partitioning of Al, W, Ti, Ta, Ni and Cr and their mutual influence was studied [5, 6]. The positive effect of Ti and Ta on stabilization and mechanical properties of the γ' phase due to their strong partitioning to γ' was established. On the other hand, Cr had a positive influence on γ' formation but a negative effect on the creep resistance, which was associated with its influence on the stacking fault energy of the γ' phase.

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SMARTMET: Utilizing Phase Instability to Design Alloys with Enhanced Mechanical Stability

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[2]Department of Computational Materials Design (CM)

In 2011, Prof. D. Raabe and Prof. J. Neugebauer were awarded an 'ERC Advanced Co-Investigator Grant', the most prestigious and competitive scientific funding in Europe. The project proposal: "SMARTMET: Adaptive nanostructures in next generation metallic materials" was embedded into the Adaptive Structural Materials (ASM) group lead by Dr. C.C. Tasan (experiments) and Dr. B. Grabowski (theory).

The main aim of SMARTMET is to address the inverse strength-ductility problem, which sets an apparent limit to the mechanical optimization of advanced engineering alloys. The basic solution approach proposed therein is the joint use of experiments and atomic-scale theoretical tools to develop new alloy design strategies based on utilizing phase instability.

A main activity combining experimental and theoretical efforts focused on designing titanium based alloys at the verge of their stability. Such ‚metastable' Ti-alloys show tremendous potential for biomedical, functional and structural applications, but exploiting the potential has so far been hindered by the intrinsic microstructural complexity revealed by these materials, as well as absence of proper guidelines in determining ideal compositions.

The theory and experimental teams have jointly selected gum metal as a starting point, an alloy with excellent properties but strongly debated micro-mechanisms, for investigating the potential for instability-based property improvement.

The experimental team has confirmed, through an extensive multi-scale characterization effort, that this alloy demonstrates multiple, previously unknown, phase transformation phenomena: i.e. a reversible nanotwinning-assisted backpack transformation from β phase to α'' and to ω (Fig. 1a).

To understand the physics of these transformations, we referred to *ab initio* simulations. The calculations lead to the fundamental understanding on the electronic scale of the phase stabilities in Ti and its alloys. Based on this knowledge and on the in parallel developed finite temperature methodology we were able to compute phase diagrams in various Ti alloys (Fig.1b). In particular, we show that at certain compositions a triple point occurs at which the phase fields of the β-ω-α'' phases are connected. This feature has important technological consequences, because it predicts compositions ranges for designing special multiphase Ti alloys.

This work is only one example of the research activities in the ASM group. There are various phase stability studies on other alloy systems, e.g. high entropy alloys, advanced multi-phase steels, Ti-alloys, etc., which demonstrate the power and the versatility of the "SMARTMET approach" of utilizing instability.

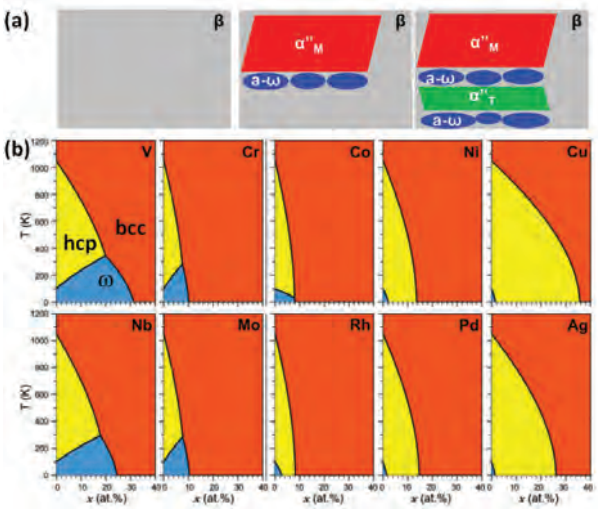

Fig. 1: *(a) Schematic representation of the nanotwinning-assisted backpack transformation phenomena; (b) Various Ti-X phase diagrams determined by ab initio simulations.*

International Network Mechanics of Nano-Objects - MECANO

G. Dehm [1], D. Raabe [2], C. Kirchlechner [1]

[1] Structure and Nano-/ Micromechanics of Materials (SN)

[2] Microstructure Physics and Alloy Design (MA)

MECANO is a multinational and interdisciplinary network, which brings together physicist, chemists, materials scientists and mechanical engineers to advance the understanding of mechanical properties of materials at small length scales. The network, which was established in 2012 by Prof. Olivier Thomas (Marseilles), is funded by the French research organization CNRS for 4 years and comprises researchers from Austria, France, Germany, Ireland, Italy, Switzerland, and UK and includes partners from universities, research institutes, large-scale research facilities, and industry. MPIE is one of the 11 European partners and actively involved in operating MECANO. G. Dehm is a member of the Scientific Committee, which meets twice a year to decide on topics of forthcoming meetings, workshops and schools. The scientific questions addressed within MECANO stretch from synthesis of nanomaterials, manipulation of their properties, to advanced experimental testing and characterization methods for quantitative determination of stress, strain, and defects down to the atomic level, questioning – as always in nanoscience – how well current theories used at the macro- and mesoscale (continuums mechanics, plasticity, elasticity theory, …) can be applied to smaller and smaller length scales. The portfolio of topics also encompasses reliability of devices and enhancement of their performance by strain engineering. The network is structured into four themes:

- Mechanics in small dimensions: elasticity, plasticity and fracture
- Experimental methods: local fields mapping and mechanical testing
- Modelling and simulation: from Ångstroms to microns
- Coupling between growth, stress and composition in nano-objects

These four topics span the core research interests of the network members and are strongly interlinked.

The complexity of the topics demands an interdisciplinary approach bringing together experimentalists and theoreticians. The strength of MECANO is the networking across discipline boundaries involving scientists across all levels of their career from graduate students to senior scientists. The MECANO network promotes scientific discussions and fosters collaborations by organizing (i) General Meetings open to all topics, (ii) dedicated Workshops on specific topics, and (iii) Schools for graduate students to review basics and put recent research developments into perspectives. MPIE organized the 2nd General Meeting from 18-19 July, 2013 with ca. 70 participants (Fig. 1). Two Schools were organized on Small Scale Plasticity (Cargese, 14-19 October 2013) and Solid Mechanics for Nanoscientists (Autrans, 17-25 March 2014) and attended by PhD students from MPIE. The international MECANO network has been very fruitful and a new funding application for the period 2016-2019 is currently compiled by the Scientific Committee.

Fig. 1: *Participants of the 2nd General Meeting held at the MPIE in Düsseldorf from 18-19 July, 2013 with ca. 70 participants including 24 PhD students and 13 postdocs.*

Steel - *ab initio* - Quantum Mechanics Guided Design of New Fe-based Materials: A Joint Initiative between MPIE and RWTH

F. Roters [2], T. Hickel [1], R. Spatschek [1], S. Sandlöbes [2], P. Choi [2], S. Zaefferer [2], D. Ponge [2], C. Scheu [3], D. Raabe [2], J. Neugebauer [1]

[1]Department of Computational Materials Design (CM)
[2]Department of Microstructure Physics and Alloy Design (MA)
[3]Nanoanalytics and Interfaces group (NG)

In 2007 the MPIE in Düsseldorf and RWTH Aachen University jointly initiated a collaborative research centre (Sonderforschungsbereich, SFB 761) on quantum-mechanics guided design of new Fe-based materials. The initiative is funded by the German Research Foundation (Deutsche Forschungsgemeinschaft DFG). Speaker and chairman of the project is Prof Wolfgang Bleck (Institute of Ferrous Metallurgy, RWTH Aachen University) and vice-chairman is Prof Dierk Raabe (MPIE). The results of the second four-year phase of the SFB 761, which ended in June 2015, were successfully presented during the evaluation of the SFB in early 2015. Based on this evaluation and the written report, a third four-year phase with seven projects executed at MPIE was granted by the DFG.

The key idea of the SFB 761 is to develop a new set of methods for materials and process design based on *ab initio* calculations in conjunction with advanced characterization and metallurgical alloy development tools. The first phase of the project focussed on the ternary Fe-Mn-C system, forming the basis of high manganese steels. During the second phase the alloying spectrum was extended to Fe-Mn-Al-C. A key quantity in the investigations was the stacking fault energy, which serves as a central link between local chemistry and engineering applications. It was used as an input in physically based strain hardening models that are fully coupled to finite element simulations. Such a multiscale approach was for example applied to investigate the crashworthiness of TWIP steel and resulted in an excellent agreement with the crash performance experimentally observed for a design component. Breakthroughs have also be achieved in the processing of TWIP steels by strip casting and in the combination of high-resolution characterization techniques such as transmission electron microscopy (TEM) and atom probe tomography (APT) to investigate for example the C segregation behaviour.

Now, in the third phase, the material spectrum is again extended towards steels with either medium Mn or higher Al content. This opens another spectrum of physical questions, where in particular phase boundaries (α/γ and γ/κ) become important. Other focus topics of the third period are strain hardening engineering and hydrogen management in these steels.

The new methods and insights developed within the SFB 761 have an impact beyond the project consortium. Within a first transfer project with an industrial partner, the tools have been applied to Fe-Cr-Mn-N-(C) steels. In the third period, a couple of further transfer projects are established. One of them, which is run by MPIE, evaluates the sensitivity of high-Mn steels that contain Cr carbides to hydrogen embrittlement. Interfaces are also of central importance in this project.

Inspired by the success of the first two periods, the SFB 761 will continue in the manufacturing and characterization of Fe-Mn-Al-C-steels of different compositions. *Ab initio* methods are not only used for the prediction of key thermodynamic parameters, but turned out to become increasingly important for understanding the ongoing mechanisms (relevant, e.g., for TWIP, TRIP, weight reduction, shear band formation and kappa-carbide formation). The aim is the quantification of the effects of chemical composition, strain rate and temperature on the occurrence and interaction of different strengthening mechanisms. The long-term perspective lies in the development of predictive and quantitative multiscale models of materials and processes that are based on *ab initio* simulations and the establishment of a new class of structural steels based on the Fe-Mn-C system.

More details on SFB761 are available on
http://www.stahl-abinitio.de

Fig. 1: *The SFB 761 team starting into the 3rd period in July 2015.*

ICAMS - Interdisciplinary Centre for Advanced Materials

J. Neugebauer [1], T. Hickel [1], R. Spatschek [1, 2], D. Raabe [3]

[1] Department of Computational Materials Design (CM)
[2] now at: Forschungszentrum Jülich
[3] Department of Microstructure Physics and Alloy Design (MA)

The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), which has been initiated in 2005 by the MPIE and has been founded in 2008, has become one of the leading institutions for scale bridging materials modelling. It includes the departments for Atomistic Modelling and Simulation (R. Drautz), Scale Bridging Thermodynamic and Kinetic Simulation (I. Steinbach), and Micromechanical and Macroscopic Modelling (A. Hartmaier). After the initial startup period of five years with substantial financial support from an industrial consortium, the state of North Rhine-Westphalia and the European Union, the institute has now become a regular unit within the Ruhr-Universität Bochum. Due to its excellent scientific performance, documented for example by its international outreach, a large number of publications, as well as a significant amount of attracted third-party funding, there is no doubt that ICAMS can successfully continue its work in the future. The MPIE has served as a strong scientific partner in this development.

Fig. 1: *Vivid discussion at the meeting of the ICAMS advisory board (headed by Dierk Raabe), with members also from the ASG Modelling from the MPIE.*

Structurally, the MPIE is embedded into ICAMS via the Advanced Study Group (ASG) “Modelling”, which supports the multiscale concept in particular at the most fundamental scale, which is dominated by electronic interactions and individual atomic processes. The success of the ASG concept has recently led to the integration of two further ASGs: Since 2012 the group “High Performance Computing in Materials Science” (G. Sudmann), which is financially supported by industry, works on the efficient implementation and parallelization of various codes developed at ICAMS. The ASG “Diffusion and Microstructure Analysis” (G. Wilde) brings in complementary experimental expertise on topics such as grain boundary diffusion, internal interfaces, as well as microstructure evolution in deformed materials.

The link between ICAMS and the MPIE is further deepened within two large-scale projects financed by the German Research Foundation (DFG) that have been attracted in the past years: Within the Collaborative Research Centre (SFB/Transregio 103) “From Atoms to Turbine” joint research on the characterization of superalloys is performed. The MPIE is further participating in the Priority Programme (SPP1713) “Chemomechanics” that is coordinated by I. Steinbach. Its associated projects investigate the interplay of mechanical and chemical forces in metals and polymers. Various other projects, e.g. within the Max-Planck Research School SURMAT, have led to an increasing amount of PhD theses that are jointly supervised by members of both institutions. Also, lectures within the ICAMS Master of Science programme “Materials Science and Simulation” (MSS) are partially held by members of the MPIE.

Due to the scientific exchange in jointly organized workshops (e.g. Ringberg Unary Workshop 2013, ADIS workshop 2014) and symposia at international conferences, common retreats, and the ICAMS Advanced Discussions, it is ensured that the close collaboration between the two institutes will also flourish in the future.

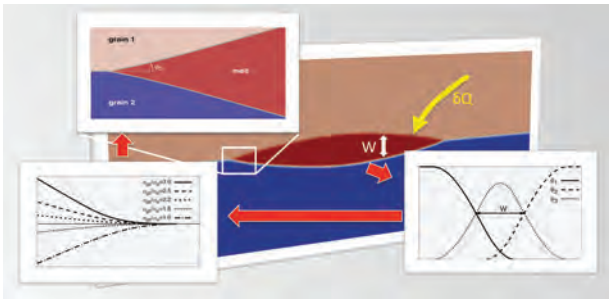

Fig. 2: *Modelling of melting along grain boundaries as a joint initiative between the department “Scale bridging thermodynamic and kinetic simulation” at ICAMS and the CM. Comp. Mat. Sci 108, 293 (2015).*

Activities within the Cluster of Excellence "Ruhr Explores Solvation" (Resolv) at MPIE

A. Erbe [1], M. Valtiner [1], F. Renner [1], M. Todorova [2], M. Stratmann [1], J. Neugebauer [2]

[1] Department of Interface Chemistry and Surface Engineering (GO)
[2] Department of Computational Materials Design (CM)

The Cluster of Excellence Resolv was established at the Ruhr-Universität Bochum (RUB) in November 2012, and is led by Prof. Dr. Martina Havenith-Newen (Physical Chemistry 2) as speaker of the cluster. Besides several departments from RUB, groups from TU Dortmund, University Duisburg-Essen, Fraunhofer UMSICHT Oberhausen, MPI für Kohlenforschung (Mülheim a. d. Ruhr), MPI for Chemical Energy Conversion (Mülheim a. d. Ruhr) and MPIE, are members of the cluster. The mission of Resolv is to establish an understanding of solvation processes at a molecular level. The cluster is structured in 3 research areas: (A) Understanding and Exploiting Solvation in Chemical Processes, (B) Connecting Solvation Dynamics with Biomolecular Function and (C) Ion Solvation and Charge Transfer at Interfaces. With their expertise in interface science, two departments GO and CM) of MPIE are strongly involved in research area C. MPIE is also involved in the coordination of the cross-linking topic "ion hydration".

So far, 5 doctoral students started their work at MPIE within the cluster's Graduate School of Solvation Science (GSS). Their projects involve surface force measurements on solvated well-defined alloy systems, preparation and investigation of "emersed electrodes", vibrational spectroscopy of solvent modes as function of electrode potential, simulation of solvated ions by *ab initio* molecular dynamics, and experimental characterisation of the defect-formation in zinc oxide. The MPIE is also involved in a number of collaborative projects of students based at RUB. Most projects with MPIE involvement call for a strong collaboration between experimentalists and theorists.

Initial results of the projects based at MPIE include investigations of the stability of polar ZnO(0001) surfaces in an aqueous environment via construction of surface Pourbaix diagrams, an accurate description of ions in solution, the setup of an experiment that enables emersion of well-defined electrodes from an electrolyte under control of the electrode potential with direct transfer to a UHV chamber, and the characterisation of the potential-dependent de-solvation of germanium after an electrochemically triggered surface termination change.

More details: http://www.rub.de/solvation

Fig. 1: *Research areas within RESOLV ((C) Ruhr-Universität Bochum).*

Max Planck Research Group on High Temperature Materials

G.Eggeler [1], A.Kostka [2, 3]

[1] Material Science and Engineering, Ruhr-Universität Bochum
[2] previously: Department of Structure and Nano-/Micromechanics of Materials (SN)
[3] Alloy Design, Ruhr-Universität Bochum

Since May 2015, Gunther Eggeler, professor for materials science at the Ruhr-Universität Bochum (RUB), leads a new Max Planck Research Group on high temperature materials (HTM), which emanated from the Max Planck Fellow Group which existed from May 2010 until May 2015. The new HTM group seamlessly continues the research activities in the area of high temperature materials. Aleksander Kostka, a scientific member of the previous Max Planck Fellow Group, is now a transmission electron microscope (TEM) scientist at the Ruhr-Universität Bochum. This position allows him to also keep an involvement in the new high temperature materials group. The expertise of the group lies in the field of exploring and explaining microstructural evolution during processing and service of engineering materials. Recently the group has contributed to a better understanding of the nucleation of the Mo-rich Laves phase during aging and creep of tempered martensite ferritic steels (TMFS) [1, 2]. It could be shown that segregation of minor alloy elements like Si to micro grain boundaries precedes the nucleation of Laves phase particles [1, 2]. As an example, Figures 1a and b show that TEM and 3D atom probe (APT) investigations (Department of Microstructure Physics and Alloy Design, MPIE) yield complementary information which is needed to identify elementary transformation and deformation processes which govern creep.

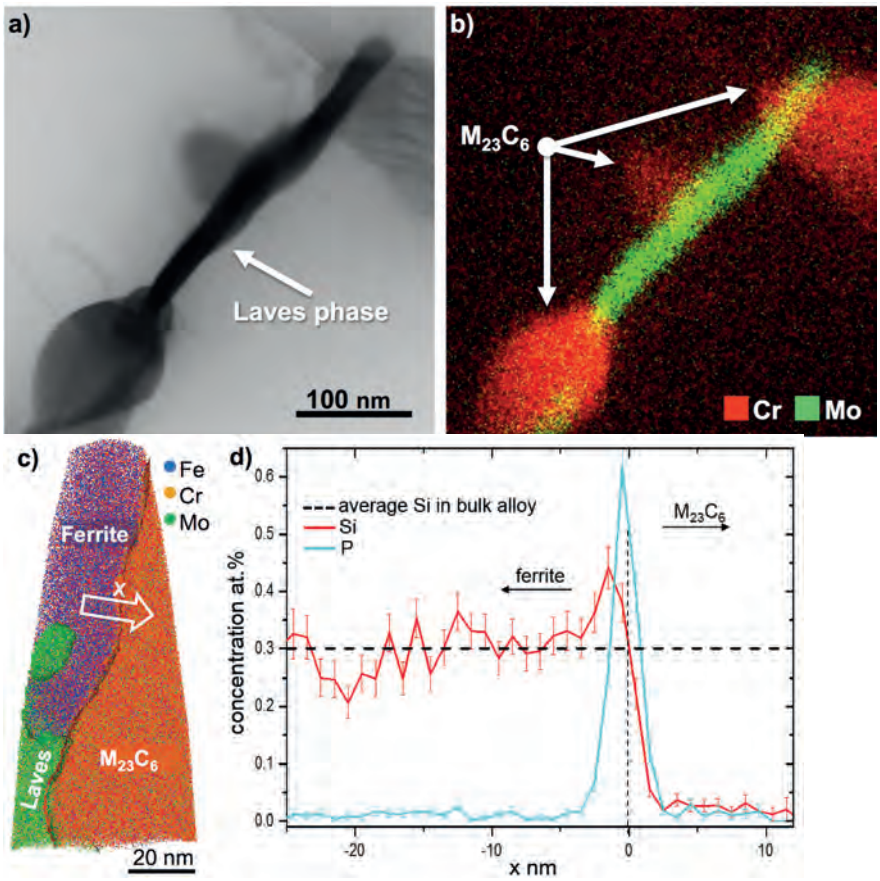

Fig. 1: *TEM/APT analyses of a 12%Cr tempered martensite ferritic steel after 82.000 hours of creep at 650°C, 120MPa. (a) Scanning TEM (STEM) bright field image showing a small Laves phase along the grain boundary. (b) Corresponding energy-dispersive X-ray spectroscopy (EDX/EDS) map of Cr (orange, highlighting carbides) and Mo (green, denoting a Laves phase). (c) APT reconstruction showing the distribution of atoms (Fe, blue; Cr, orange; Mo, green). Violet, orange and green regions denote ferrite, $M_{23}C_6$ and Laves phase, respectively. White arrow marks the positions of the concentration profile plotted in (d). (d) Concentration profile of Si and P along x axis.*

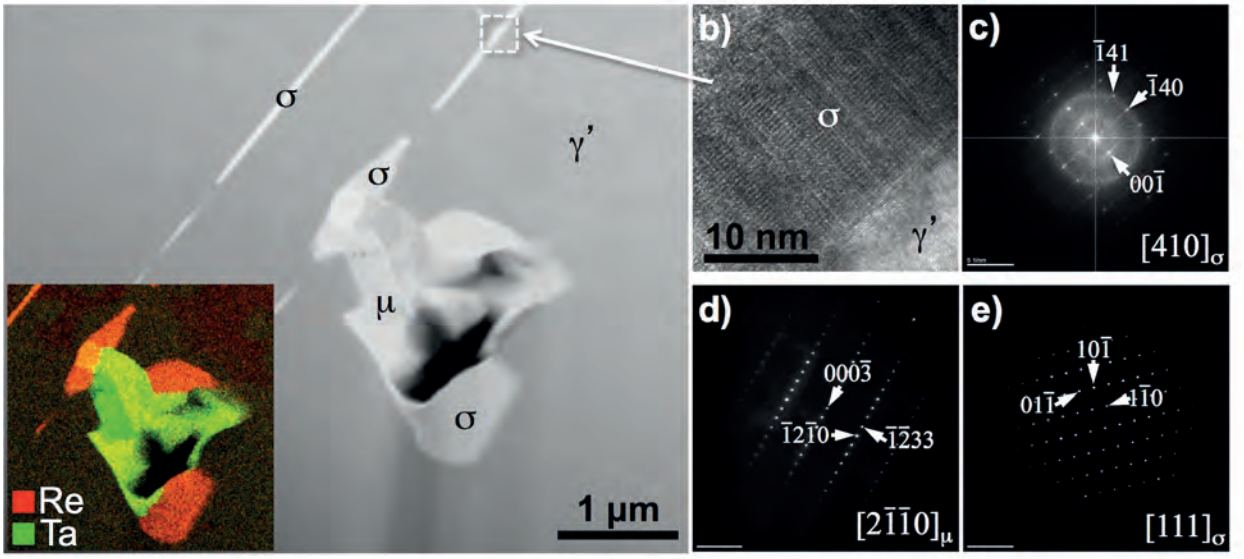

Fig. 2: *TEM analysis of precipitations in Ni-base superalloy ERBO/1 after 1000°C, 32 h heat treatment. a) STEM HAADF (high-angle annular dark field) micrograph with an EDS inset showing the distributions of Re and Ta; b) High resolution TEM (HRTEM) micrograph of the needle-like σ-phase precipitate and c) corresponding FFT; d) and e) characteristic selected area diffraction patterns taken from σ and μ-phase, respectively.*

The HTM group also performs research in the area of single crystal Ni- and Co-based superalloys. The HTM group organized collaboration between several partners which yielded a full microstructural characterization of a Ni-base superalloy, addressing macroscopic, mesoscopic and atomistic phenomena [3]. There was also an effort to study the thermodynamics and kinetics of TCP phase formation during high temperature exposure [4]. As an example, Fig. 2 shows a TEM analysis of precipitations in Ni-base superalloy ERBO/1 after 1000°C, 32 h heat treatment where σ-and μ-phase are clearly distinguishable. The needle-like σ-phase forms initially in the {111} γ-phase habit planes as can be observed in Fig. 2a or more clearly in Fig. 2b and c. The σ-phase consists of Cr, Mo and small fraction of Re, while μ-phase - mainly of Hf and Ta. At 1100°C the σ-phase seems to be not stable: precipitates are found only after short heat treatments while they disappear after 50 h annealing time. At 1200°C, no precipitates of the σ-phase form at all, regardless of the annealing time.

In the superalloy field, HTM acts as a link between MPIE researchers and materials researchers at other affiliations (Universities of Bochum and Erlangen, Deutsches Luft- und Raumfahrtzentrum and Forschungszentrum Jülich). For the future it is planned to continue the successful collaboration with the MPIE departments of Dierk Raabe and Gerhard Dehm, combining the group's expertise in high temperature materials with *in-situ* TEM experiments (Dehm department) and the 3D atom probe (Raabe department). Emphasis will be placed on the improvement of existing and the development of new high temperature materials. Moreover, new advanced topics like high temperature shape memory alloys, high entropy alloys and microstructural evolution during additive manufacturing will be tackled.

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Research Funding

K. Hübel

Professional Support in Research Funding

In the reporting period 2013-2015 Dr. Katja Hübel provided professional support in national, European and international research funding to the scientists of the MPIE with the aim of increasing the success of funding applications. She started working at the MPIE in February 2013 and gave advice on all kinds of funding from individual (e.g. Humboldt Research Fellowship for Postdoctoral Researchers, Marie Sklodowska-Curie Individual Fellowship and ERC Grants) to project funding (e.g. Horizon 2020, German Ministry for Science & Education and German Research Foundation). Furthermore special attention was drawn to prizes and awards (e.g. Leopoldina Preis, Adolf-Martens-Preis and deutscher Studienpreis). Support in research funding was oriented on the strategic development of the MPIE as well as on its interdisciplinary research focus.

Competitive Applications

Professional and administrative assistance was provided for researchers throughout the whole process of application. Support was given in identifying the right funding scheme fitting to the scientific profile or project needs, in proposal writing as well as in budget calculation. For networking projects coordination of the project partners was offered.

Project Management

Support in project management was also given. This included assistance in setting scientific project reports as well as in financial reporting. Project reporting was done in close collaboration with the MPIE administration.

Support for Junior Scientists

In the current reporting period 2013-2015 a special focus was set on young scientists. This included not only finding the right funding scheme that fits to their scientific profiles but also strategic advice for their career development. Furthermore a workshop "Competitive Proposal Writing" has been given for the first time in summer 2015 and will be offered in yearly intervalls. Another workshop "Applying for ERC Starting & Consolidator Grants" is organized yearly with the MPI for Radioastronomy in Bonn and with the National Contact Point ERC. This workshop is a special offer to junior scientists at Max Planck Institutes in North Rhine-Westphalia. Support was given to junior scientists working at the MPIE as well as to prospective junior scientists planning to work at the MPIE.

Fig. 1: *Dr. Pascal Beese (right) received the Leopoldina Prize for Junior Scientists. Left: Prof. Jörg Hacker, President of Leopoldina. © Christof Rieken, Leopoldina*

Selected Research Funding

Dr. Blazej Grabowski got an *ERC Starting Grant of the European Research Council*, Horizon 2020, "Time-scale bridging potentials for realistic molecular dynamics simulations-TIME-BRIDGE", *ERC* Jul 2015 – Jun 2020.

Dr. Markus Valtiner got the *„Max-Buchner-Forschungsstipendium"* starting in Jul 2014

Dr. Karl Mayrhofer won the *Dechema-Preis der Max-Buchner-Forschungsstiftung*, Nov 2014

Christian Broß won the *Apprentice Prize of the Max Planck Society*, Jul 2015.

"International Max Research School (IMPRS) for Surface and Interface Engineering in Advanced Materials (SurMat)", Follow-up application, *Max Planck Society*, Jan 2016 – Dec 2020.

"Enhanced substrates and GaN pilot lines enabling compact power applications – PowerBase", *The ECSEL Joint Undertaking, FP7*, May 2015 – Apr 2018.

Dr. Raheleh Hadian (Iran), McMaster University Hamilton/Canada, *Humboldt Research Fellowship for Postdoctoral Researchers*; Mar 2015 to Feb 2017.

PhD Representatives

C. Baron, P. Bhogireddy, V. Dandapani, S. Hieke, Z. Li, W. Luo, A. Wengert

The PhD representatives are the interdepartmental representation of the PhD students at the Max-Planck-Institut für Eisenforschung (MPIE) GmbH. All PhD students at the MPIE elect once a year seven representatives, one or two per department. The target of the representatives is to maintain and further develop the interdisciplinary cooperation and exchange of PhD students. They also serve as connection to the PhDnet, a platform for exchange among doctoral students of all Max Planck Institutes and provide their fellow colleagues at the MPIE with up-to-date information about stipend and contract possibilities, insurance information and other upcoming topics.

Fig. 1: *Career talk with BASF on 18 November 2015.*

Further, the PhD representatives initiate and organize soft skill courses for PhD students on a regular basis with topics such as scientific writing, presentation and leadership skills. Additionally, career talks are organized to give PhD and postdoctoral students a chance to build up industrial contacts and to get an insight about job possibilities in different industrial branches. In 2015 career talks with the participation of the companies ThyssenKrupp Steel Europe, McKinsey and BASF received highly positive feedback. With the goal of improved knowledge transfer in the Institute, the representatives also launched a lecture series in 2015 on important scientific tools and techniques which are of general interest to them. Examples were introduction to Matlab and electron backscatter diffraction. The events and courses received a lot of positive response from the PhD students in the Institute and will be continued.

Fig. 2: *Networking at the first career talk held at the MPIE with guest speakers from ThyssenKrupp Steel Europe.*

Alumni Networking

B. Kohlhaas

Working at the MPIE has significantly influenced the career of many scientists. Over the years, a considerable number of employees have worked at the Institute in various fields and departments. To encourage a lively exchange among the former Institute members, the alumni network has been established in our Institute in 2003 and has 300 members at present.

What does "Alumni" mean?

The word "alumnus" is derived from the Latin "alere", "to nourish", and means "nursling" or "pupil". "Alumni", the plural form of "alumnus", literally means "the nurtured ones". In the USA, the term "alumni" has been used for graduates or former students of institutes of higher education for more than 200 years. In Germany, it is only since the last few years that alumni activities are being established at universities and research institutes. (www.wikipedia.de)

Who are Alumni?

Alumni are all former staff members of the MPIE who worked at the Institute for more than six months, regardless of whether they worked here as a scientist or technician, in the workshops, library, or administration.

What are the aims of the Alumni Network?

The Network cultivates contact and shares experiences. A major intention is to establish a platform for discussions of common interests and problems, and for sharing both professional and personal experiences.

Keep in Touch

The alumni network will help not only to stay in contact with former colleagues, but also to forge new links with current Institute members, thus supporting an active and beneficial exchange for all.

Members of the alumni network will be kept updated about news, events and actions of the MPIE by mail or e-mail.

Special alumni meetings with scientific lectures and a full social programme allow members to meet colleagues, share experiences and forge ties that may lead to new collaborations.

In addition, you can inform yourself about Alumni News and easily join to the Network online https://alumni.mpie.de

Alumni Meeting 2014

Our last Alumni Meeting, "Applied fundamental research for nearly 100 years", took place at MPIE on 28 May 2014 on the occasion of the 60th Birthday of Prof. Martin Stratmann.

180 guests, including alumni and current MPIEemployees, attended the successful event.

Fig. 1: *Networking at the Alumni Meeting 2014.*

Fig. 2: *Prof. M. Stratmann giving a speech at the Alumni Meeting 2014.*

The Institute in Public

Y. Ahmed Salem

Public Relations

The reporting period 2013-2015 was full of events and changes for the Public Relations (PR) of the MPIE. A communication strategy with defined target groups and a portfolio of different methods and measures to reach the defined target was developed. The current reporting period was characterized by the implementation of the different measures. Here, the PR mainly concentrated on two sections: the “traditional” press relations on the one hand including a website relaunch in May 2015, and event management on the other hand.

Event Management

Besides various tours through the Institute and its laboratories for pupils, students, interested groups out of the broad public and for politicians and industrial partners, some major events took place in the years 2013-2015. Some of them will be presented in the following:

Science Days at the Theodor Fliedner School, February 2013 and 2014

Once a year the Theodor Fliedner School organizes the so-called Science Days where companies and institutions either visit the school and present their work or invite interested pupils to their facilities. The PR regularly takes part in this event and either organizes lab tours through the Institute or trains doctoral students to give an interactive talk with small experiments to the pupils at the school. The talks in 2013 and 2014 were held by Tom Jäpel and Emanuel Welsch, doctoral students in the department Microstructure Physics and Alloy Design (MA).

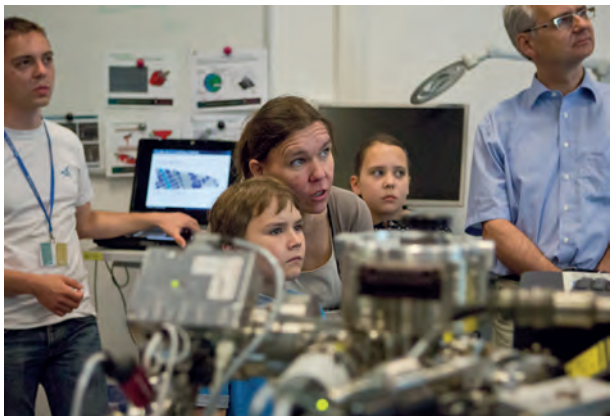

Fig. 1: *In the laboratory of the atom probe during the Open Day 2013.*

FameLab, March 2013

Fady Archie, previously master student and now doctoral student in the MA, was coached by the PR to participate at the FameLab 2013, a science slam competition. Archie won the competition for North Rhine-Westphalia and had the chance to take part at the competition in Berlin, where all winners of the German states took part. There he made the second place.

Fig. 2: *Dr. Markus Valtiner, group leader in the Department of Interface Chemistry and Surface Engineering (GO), while explaining his research during the Researchers’ Night 2013 in Düsseldorf.*

Open Day, July 2013

Together with the Steel Institute VDEh, the MPIE organized an Open Day in the summer of 2013 which attracted over 2500 people. The programme comprised over 30 different MPIE attractions showing the research in different ways to young and old.

Düsseldorfer Tage der Berufsorientierung – Days of Career Orientation, July 2013

The career orientation days in Düsseldorf were organized mainly by the City of Düsseldorf and the Chamber of Commerce and financially supported by the European Union and the Federal Ministry of Labour and Social Affairs. Pupils had the chance to spend one day at the MPIE and get an insight into the different research areas as well as the various apprenticeship possibilities at the Institute.

Researchers‘ Night in Düsseldorf, September 2013 and 2015

The first Researcher’s Night in Düsseldorf was organized 2013 by the Heinrich Heine University Düsseldorf and the University of Applied Science Düsseldorf and took place in various locations all over the city. The PR organized the MPIE’s participation with attractions in three fields: energy and environment; technology and medicine & technology and society. The Researchers’ Night 2015 took place in the heart of the City Düsseldorf, where the PR and doctoral students of different departments presented research results on TiNb hip implants and additive manufacturing, to a broader public.

MS Wissenschaft, Mai – September 2014

In 2014 the MPIE took part at the MS Wissenschaft, an exhibition ship which serves as a floating science centre and cruised from May till September 2014 in around 40 cities in Germany and Austria. This exhibition is supported by the Federal Ministry of Education and Research. Its topics match the current Science Year’s topic which is proclaimed by the Ministry. The “Ageing Society” was the central theme in 2014, where the PR presented the work of the department of Computational Materials Design (CM) on TiNb hip implants and on computer simulations being an important pillar in modern alloy design.

KopfSalat, since September 2014

KopfSalat is a new event taking place twice a year at the Institute and inviting researchers of different research areas to give generally understandable talks to the broad public of Düsseldorf. The intention is not to give an insight on the MPIE research but to attract people to come to the Institute by offering different research topics. The PR invited Prof. Dr. Martin Wikelski from the Max Planck Institute for Ornithology, Radolfzell, as the guest speaker of the first KopfSalat event in September 2014. Prof. Wikelski explained how animal migration can be used as a warning system for natural catastrophes and how he is working to build up a satellite supported system to do so. This event attracted around 70 visitors who entirely subscribed to the PR mailing list to be informed regularly about public events taking place at the MPIE.

Fig. 3: *KopfSalat invites twice a year researchers of different research areas to give generally understandable talks at the MPIE. This is an impression of the second event in April 2015.*

The second KopfSalat event attracted about 92 visitors and was led by Prof. Hanns Hatt, professor and researcher in the field of cell physiology at the Ruhr-Universität Bochum. He explained how smelling functions, how this is influenced by hormones and how everyone can influence other people’s perception by using different odours.

The third KopfSalat was at the end of November 2015. This time Prof. Gerd Gigerenzer from the Max Planck Institute for Human Development, Berlin, was invited to give a talk on adaptive behaviour and cognition. The event was visited by 120 persons.

The PR chooses the various speakers mainly out of the winners of the Communicator Prize of the German Research Foundation. This prize is awarded once a year to researchers who are especially able to present their work in a generally understandable and entertaining way. To attract as many visitors as possible to KopfSalat, the event is announced in the local newspaper, different online and social media sites and through post cards which are distributed in the neighbourhood of the Institute, at the Heinrich Heine University Düsseldorf and at the Adult Education Centre Düsseldorf.

Fig. 4: *Sample Preparation at the Girls‘ Day 2015.*

Girls‘ Day, April 2015

A group of girls had the chance to get an insight on the work of a Max Planck scientist on 23rd April 2015, the nationwide Girls’ Day. At the Girls’ Day companies, universities and different organizations invite female pupils once per year for one day. The girls learn about possible trainings and courses of study in fields usually dominated by men like IT, craft, natural sciences and engineering. The girls were supervised by doctoral students of the Max Planck Research Group Nanoanalytics and Interfaces and examined different samples with light microscopes and a scanning electron microscope.

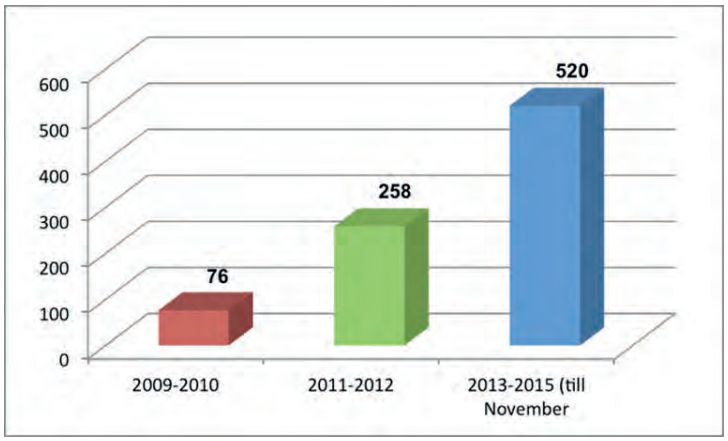

Fig. 5: *Comparison of absolute amount of clippings during different reporting periods.*

Press Relations

The Institute was mentioned 520 times in newspapers/journals and websites and 39 press releases were written during the reporting period (till 1rst of November). These are more than four times more clippings compared to 2009-2010 and a plus of 25% compared to the last reporting period 2011-2012.

Selected articles published in different print and online newspapers and journals:

20th October 2013 Frankfurter Allgemeine Sonntagszeitung: Damit er nicht so schnell kaputtgeht

27th November 2013 Rheinische Post: Düsseldorfer Forschung führt in die ganze Welt

17th March 2014 Welt der Physik: Reale Materialien aus dem Computer

5th November 2014 Die Welt: Atomsonden erforschen Nanostrukturen

5th February 2015 Spiegel Online: Hochfest und Leicht – Nanokristalle formen den Superstahl

23rd March 2015 Springer Professional: Symphonie im Stahl

The **MPIE newsletter** as a specific tool to reach the industrial partners and other publics interested in materials science, was restructured. Compared to former editions which covered different topics per release, the newsletter now focuses on one topic each, as e.g. the edition 01/2015 which is about hydrogen embrittlement. This way important topics of the Institute's interdepartmental research are highlighted and the interdepartmental research activities are better shown.

The **website of the MPIE** was relaunched in May 2015 including a complete new backend system, layout and structure. The layout is based on the corporate identity of the Max Planck Society to have a better brand recognition. The website is now structured to reach the different target groups of the Institute like scientists but also industrial partners, journalists and the broad public. Therefore, it contains all basic information both in German and in English.

Fig. 6: *The MS Wissenschaft is a floating science centre where the MPIE presented how simulations can help in developing better him implants. Copyright: Ilja Hendel, Wissenschaft im Dialog*

Internal communication and new communication tools

The MPIE Intranet was further developed by adding information on child care, business travel, living in Germany, funding and events taking place in and outside the MPIE. It is now a first address especially for newcomers to inform themselves about internal matters. In the future it will also contain all regularly required forms and templates like flexitime sheets.

The PR has also designed a MPIE calendar with scientific eye-catching images as a new marketing and communication tool. Since 2014 the calendar is distributed to industrial partners, journalists and visitors. It gives an impression on the variety of research topics at the Institute.

PART II.

THE DEPARTMENTS

(in alphabetical order)

Department of Computational Materials Design

J. Neugebauer

Scientific Objective and Department Structure

One of the major challenges to **simulate advanced materials** such as steels is their **structural, chemical and thermodynamic complexity** together with the fact that they are in realistic scenarios not isolated but in **an (often reactive) environment**. Most of the presently available simulation techniques address only a small part of this complexity and are restricted to a specific length scale. The objective of the department is the **development of computational tools and strategies that are capable to deal with realistic materials and processes**, the application of which allows a close link to the experimental activities in house and of collaborators worldwide.

Achieving this goal requires novel **scale bridging multi-scale approaches** that link fully parameter-free *ab initio* calculations with technologically relevant materials properties as well as strategies to push the predictive power and the computational efficiency of existing methods to their limit. These methodological developments and applications in the CM are performed in six groups headed by internationally highly visible scientists. The specific topics of the groups have been chosen such that their respective methods, expertise and investigated materials are complementary and can be linked in order to address material classes and questions that escape a single method. The availability of these methods opened a very productive route to study for example the complex phenomena that control the mechanical behaviour of ultra-high strength, TWIP (twinning induced plasticity), TRIP (transformation induced plasticity) or pearlitic steels (see p. 183).

It further provided a close link to interpret or guide experimental activities such as, e.g. electron microscopy (department of Structure and Nano-/Micromechanics of Materials (SN) and the independent research group Nanoanalytics and Interfaces (NG)), atom probe tomography (department of Microstructure Physics and Alloy Design (MA)) or Kelvin probe technique (department of Interface Chemistry and Surface Engineering (GO)) (see p. 149). In this way industrially relevant material science questions such as electrochemistry (see p. 161), tribology (see p. 179), grain boundary embrittlement (see p. 173) and hardening in Mg alloys (see p. 141) have been addressed in collaboration with the other departments.

Fig. 1: *The CM (summer 2015).*

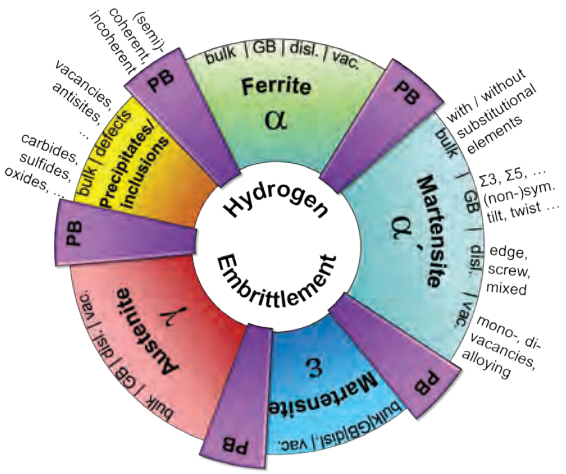

Fig. 2: *The spectrum of microstructure features that can interact with hydrogen and are therefore considered in the simulation of hydrogen embrittlement performed in the CM.*

The synergy between the groups within the CM is important to solve multi-scale problems such as hydrogen embrittlement (see p. 39), an effect that is strongly hampering the application of modern ultra-high-strength steels. Here, a complete picture of the detrimental effects of hydrogen (Fig. 2) could only be achieved by combining (i) the systematic and extensive *ab initio* study on its interaction with microstructure features such as vacancies, grain boundaries, precipitates in T. Hickel's group (Computational Phase Studies) with (ii) the atomistic description of plasticity related processes such as the hydrogen impact on dislocations and dislocation loops in B. Grabowski's group (Adaptive Materials) and (iii) the continuum investigations on the role of surface or interface strains on the solubility of hydrogen in R. Spatschek's group (Mesoscale Simulations). Linking these activities and results provided a unique insight into the various stages of hydrogen embrittlement and delayed fracture and allowed highly productive collaborations with experiments in house (MA, GO), with industry (e.g. projects funded by the European Commission such as HYDRAMICROS coordinated by T. Hickel), large scale research projects such as the DFG Collaborative Research Centre (see p. 52) or with other theory groups (see p. 53).

A key to successfully addressing this wide range of scientific questions was the strong methodological expertise that has been built up in the department over the last reporting periods. Only the availability of this expertise on advanced and highly accurate electronic structure calculations and their combination with thermodynamic, mechanical or chemical concepts enabled novel approaches and strategies that include contributions and mechanisms relevant in real materials, but that so far were impossible to compute with existing *ab initio* approaches [1]. One such example is a new formalism (see p. 177) for a fully *ab initio* description of magnon-phonon coupling, i.e., the effect magnetic excitations have on atomic vibrations and thermodynamic stability at higher temperatures [2]. By combining Spin-Quantum-Monte-Carlo methods with the spin-space-averaging (SSA) approach developed by the department in the previous reporting period, it became possible to understand this mechanism and to achieve an accuracy that agrees well with experiment. Since this effect is the major cause of the high temperature softening of ferritic steels, our insights can support the efforts in the MA to improve the mechanical properties of such steels. Other examples of novel methodological approaches that have been achieved based on the systematic developments of the last years are a highly efficient concept of computing anharmonic free energy contributions [3] that opens the route towards routinely including them in *ab initio* calculations or a generalization of the widely used Arrhenius concept to describe point defect concentrations [4]. The latter revealed that previously accepted and in compilations listed defect formation energies have to be revised by 10-20%. These methodological developments have been achieved by combining the expertise of T. Hickel's and B. Grabowski's group and have been published in top journals in the field (Phys. Rev. Lett., Phys. Rev. X).

Next to the long term development of *ab initio* based thermodynamic approaches, a major strategy in the last period was to use the broad materials expertise of the department, ranging from steel related systems over oxide/semiconductor topics to biomimetic materials, to link fields that so far were methodologically not connected. An example in this respect is the transfer of defect concepts that are well established in the semiconductor community to electrochemistry in the group "Electrochemistry and Corrosion Sciences" headed by M. Todorova. This "translation" made the concepts useful for both communities and allowed to use extensive sets of point defect calculations performed in semiconductor physics to understand corrosion of protective oxide layers. For example, this approach revealed that neutral oxygen vacancies rather than charged vacancies as always assumed in electrochemistry are relevant for the growth of the protective oxide layer [5]. Another example for a successful link of two different fields is the development of an analytical approach with atomistic resolution by G. Leyson (Humboldt Fellow) that connects mechanical and thermodynamic concepts and allowed to derive phase diagrams for defect-induced nanostructure phases [6]. Further, C. Freysoldt's and L. Lymperaki's groups combined statistical mechanics concepts and growth simulations [7, 8].

To keep the expert knowledge despite the rapid and desired fluctuations of key scientists in the de-

partment, we continued the development of a Python based workbench called “Pyiron” that combines all aspects of setting up complex simulations, performing accurate convergence tests and error analysis, handling large amounts of computer runs with advanced databases and visualization. This toolset allows to “conserve” the methodological expertise of the various groups by generating automatized simulation protocols and by guaranteeing the targeted high numerical accuracy. A new generation of Bachelor, Master and PhD students in the department used Pyiron to handle projects consisting of several $10^4 \ldots 10^5$ jobs that would have been hard to control and analyze with existing methods. Examples where the tool has been successfully used are the identification of chemical trends of interstitials in metals by using concepts of machine learning [9] or the calculation of TTT (Time-Temperature-Transformation) phase diagrams, which are crucial for the control of precipitates in steels and whose complete derivation with atomistic concepts has not been reported in the literature before [10].

The scientific results were also made available to the community by many publications in high-ranking journals. In the reporting period the H index of the department has increased by 66% (15 → 25). Here, our review papers, e.g., on first-principles calculations for point defects in solids [11] or lambda-transitions in materials [12], as well as our interdepartmental collaborations, e.g., on TWIP-steels [13] and Mg alloys [14] encountered the greatest interest in the field.

To further stir and disseminate these developments in the scientific community, the scientists in the department have been very active in organizing and co-organizing key conferences and symposia. One highlight was the now 5th ADIS (*Ab initio* Description of Iron and Steels) symposium which was organized by T. Hickel and attracted again the international top experts to Ringberg Castle. He also successfully co-organized the Unary Workshop (Fig. 3) that brought together the CALPHAD and the *ab initio* community [15]. The department further organized symposia at leading materials science and physics conferences (see p. 219). The CM also successfully run small and highly focused meetings in emerging fields that were very well received by the community: For example, S. Hadian and B. Grabowski organized a meeting on grain boundary migration in Günzburg and M. Todorova and C. Van de Walle (UCSB) a meeting on bridging electrochemistry with semiconductor defect chemistry in Santa Barbara. Members of the department are also actively involved in representing the community: J. Neugebauer has been elected head of the division Metals and Materials in the DPG and as representative (Fachkollegiat) in the Theoretical Chemistry Division of the German Research Foundation (DFG) and became editor of a newly established Journal of the Nature Group (Computational Materials). We are also closely connected to the neighbouring universities in Bochum, Aachen, Duisburg-Essen and Paderborn by large scale joint projects and activities such as the Interdisciplinary Center of Advanced Materials Simulations (ICAMS; see p. 53), the International Max Planck Research School SurMat (see p. 47 (with J. Neugebauer as speaker) or teaching duties (see p. 230).

The high scientific reputation that members of the department receive is reflected by the large number of invited and keynote talks at the major international conferences in the field. Members of the department also received prestigious prizes: B. Grabowski got an ERC starting grant, B. Lange the Otto-Hahn medal for an outstanding PhD thesis or G. Leyson and S. Hadian a Humboldt research fellowship. It is also reflected in changes in the group structure since

Fig. 3: *The Ringberg Unary Workshop 2013 was one of several workshops organized by the CM in the reporting period. It was devoted to fundamental concepts of computational thermodynamics.*

leading scientists got prestigious offers at institutions worldwide. M. Friák, who from the beginning of the department had headed the very successful group "*Ab initio* thermodynamics", is now the leader of a large experimental and theoretical group at the Academy of Sciences of the Czech Republic. R. Spatschek, has built up over the last five years a highly productive group on Mesoscale Simulations that linked many of the atomistic concepts of the department to experimental activities. He accepted an offer on a joint professorship position at the Research Center in Jülich and the RWTH Aachen, which he started October 1st, 2015. The scientific expertise is kept up by maintaining strong links with these and other leaving scientists via joint projects and publications. Furthermore, a new research group "Electrochemistry and Corrosion" has been created and is headed by M. Todorova starting October 1st, 2015 (see p. 28). This group will provide a strong link to the activities in the GO, particularly to the groups of S. Wippermann, M. Valtiner and A. Erbe, but is also connected to the semiconductor/oxide activities in C. Freysoldt's group as well as to the thermodynamic sampling concepts in T. Hickel's and B. Grabowski's groups. L. Lymperakis became a project leader in a large EU project and heads the project group "Growth Modeling" that addresses a wide range of semiconductor related activities. In the following the group activities are briefly summarized:

Research Groups

Computational Phase Studies (T. Hickel)

This group is devoted to the physics of (meta) stable thermodynamic phases in metals as well as transitions between them. Its major vision is an *ab initio* based prediction of thermodynamic properties and bulk phase diagrams, being directly related to many technologically relevant mechanisms in metals. According to the spirit of the whole department outlined above, the group made in the reporting period substantial progress developing methods for an application to advanced material systems such as:

- The improvement of *ab initio* based methods to calculate anharmonic contributions to the free energy of metals caused by the interaction of phonons and of lattice and magnetic degrees of freedom. [2, 3]
- The comparison of *ab initio* determined thermodynamic properties with experiments and their combination with thermodynamic databases. [4, 16]
- The description and prediction of temperature and stress induced phase transitions and/or structural changes in shape memory alloys, steels and related materials. [17, 18]
- The energetics and kinetics of alloying elements, impurities and defects, and their relevance for embrittlement phenomena, precipitation and ductility of materials. [19, 20]

All these activities are characterized by **strong collaborations** with other groups in the CM, with other departments of the MPIE, as well as with academic and industrial partners in various research institutions. The Ringberg Unary workshop 2013, which was organized by T. Hickel, U.R. Kattner (NIST, USA) and S.G. Fries (ICAMS, Bochum), is a consequence of the world-wide interaction in computational thermodynamics (Fig. 3). It addressed the most promising concepts to improve the accuracy and physical fundament of thermodynamic databases regarding crystalline phases, liquid phases, lambda transitions in materials, effects of pressure and stress, and point defect thermodynamics [15]. As outlined in five large review articles (e.g., [12,21]), which came out of this workshop, the recent progress in combining *ab initio* calculations with thermodynamic concepts pushed the insights and achievements substantially forward for each of these topics. The group has continuously contributed to this development.

Anharmonic lattice vibrations, for example, form a particular challenge for the description of the crystalline state of materials at finite temperatures. We revealed that the asymmetric nature of the local potential for the nearest-neighbour atomic interaction provides the underlying physics for these excitations (A. Glensk, see also p. 171). Based on this insight, a highly efficient approach was developed and benchmarked for an extensive set of unary fcc metals [3]. Astonishingly, this study revealed that anharmonic heat capacity contributions can be of the same order as the quasiharmonic corrections due to thermal expansion.

Consequently, anharmonic lattice vibrations have also been taken into account for the Gibbs **energy of vacancy formation** in Al and Cu (A. Glensk). The resulting highly nonlinear temperature dependence in the Gibbs formation energy naturally explains experiments and shows that nonlinear thermal corrections are crucial to extrapolate high-temperature experimental data to T = 0 K [4, 11, 21]. The findings are related to the observation that the formation entropy of vacancies is not constant as often assumed, but increases almost linearly with temperature.

The treatment of **magnetic excitations** within the scope of phase studies is another field of central interest, since its complexity and numerical challenge requires non-trivial solutions. We have developed a set of analytical and numerical methods, how in particular the quantum-mechanical character of this free energy contribution can be taken into account [22] and have applied them to magnetic elements, including Cr [16]. It is typically assumed for the computation of phase stabilities that an adiabatic decoupling of entropy contributions is present [12]. In the last years we realized, however, the importance of a magnetically driven modification of lattice vibrations not only in the paramagnetic limit, but already close to the ferro- to paramagnetic transition (F. Körmann, see also p. 177). Our developed temperature-dependent spin-space averaging (SSA) technique has led to phonon spectra that are in perfect agreement with recent sophisticated experimental findings [2]. Related approaches have also been developed to describe the magnetic influence on structural parameters such as stacking fault energies (I. Bleskov) [23]. In an alternative approach based on the itinerant coherent potential approximation, we additionally checked the impact of magnetic fluctuations on these results and found them to be small [24].

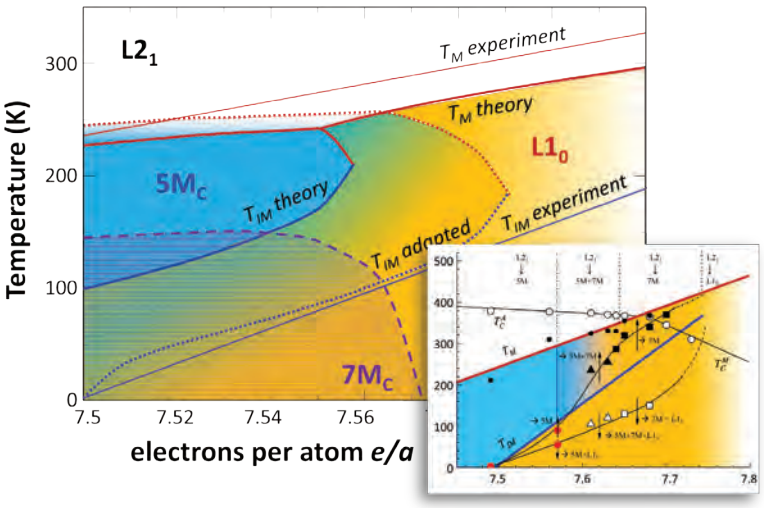

Fig. 4: *Ab initio calculated phase diagram of $Ni_2Mn_{1+y}Ga_{1-y}$. The martensitic transformation T_M (thick red line) separates the austenite from different martensitic phases. The theory predicts an intermartensitic transformation T_{IM} (thick blue line) between the 5M phase (blue-coloured area) and the $L1_0$ phase (orange). For comparison the experimental results are shown by thin lines and in the inset. The stability region of the commensurate 7M is indicated by a purple dashed line. Figure adapted from [25].*

The investigations on **Heusler alloys** underline the need for accurately determined free energies. In the reporting period the presence of intermartensitic transformations in Ni-Mn-Ga alloys was a key question, due to the major importance for shape memory and magnetocaloric effects that make the material class interesting for applications (B. Dutta). Here, tiny energy differences between structures that only differ in small modulations are present. The successful clarification of experimental uncertainties not only about the chemical trend, but also about the physical origin of such transformations, is therefore a highlight of the present research activities (Fig. 4) [25]. The investigations of martensitic phase transformations have meanwhile even been extended to quaternary Heusler systems [17]. In collaborations with experimental partners within the DFG priority programme SPP1599, also other interesting phenomena of this material class have been explained by *ab initio* investigations [26, 27]. A rather surprising outcome was the identification of Heusler phases as precipitates in steels [28].

The free energy of formation of certain phases has besides cementite in steels (F. Körmann) [29] been further investigated for various **structural materials with high-potential for applications**, including the Q phase in Al alloys for light-weight constructions (A. Zendegani) [30], Laves-phases in Fe-Nb alloys for high-temperature energy applications (A. Zendegani), and various phases in Nd-Fe-B and Ce-Fe-Ti for hard-magnetic materials (H. Sözen).

In these studies we realized that a pure thermodynamic argumentation is often not sufficient to explain the experimentally observed formation of secondary phases. In particular in steel microstructures the **interfaces to the matrix material** can be of key importance for the precipitate structure and chemical composition. In the case of κ carbides (see p. 149), for example, we revealed that the elastic energy due to misfit strain explains a substantial deficiency of carbon in the precipitate phase (P. Dey) [31]. The situation is even more complicated in the case of cementite, when it forms at the interface between austenite and ferrite in a coupling process (X. Zhang). This is because three phases and a combination of the martensitic rearrangement of Fe atoms and a diffusion-driven separation of C atoms are simultaneously present. We have shown that a metastable intermediate structure (MIS) in the spirit of complexions can serve as a natural link between these phases and can explain the atomic process during decomposition (Fig. 5) [18].

Treating the interplay of nanodiffusion and structural properties was also decisive for the simulation of **mechanical properties** in high-Mn steels (I. Bleskov). The stacking fault-carbon interaction in

these steels is characterized by an anti-Suzuki effect, i.e. the interstitial C atoms will diffuse away from the planar defect. Since the relevance of this process depends on the temperature imposed by the experimental conditions, we were able to explain different chemical trends observed in experiment [20]. These insights into atomic mechanism are decisive for an *ab initio* based prediction of deformation behaviour, e.g. the crash performance of modern steels [32] and have contributed to the success of the collaborative research centre SFB 761 "Stahl – *ab initio*" and its extension by another funding period starting in 2015.

A kinetic investigation of the precipitate formation has been performed for Al-Sc using **kinetic Monte-Carlo simulations** (A. Gupta) within the DFG priority programme SPP1713. The highlight of this work was the prediction of general features in

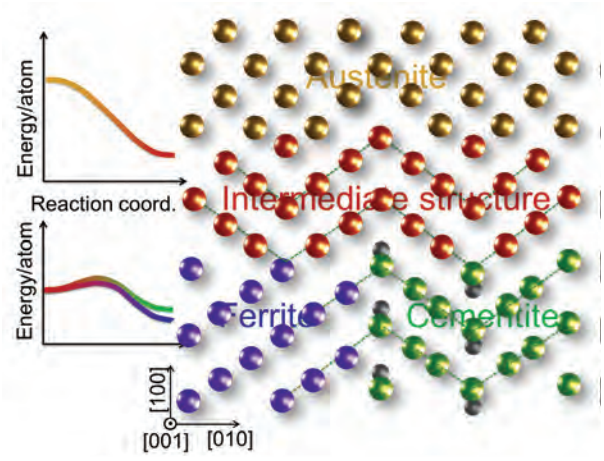

Fig. 5: *Representation of the atomistic mechanism of austenite decomposition including the effect of interfaces. Large spheres refer to Fe atoms in austenite (gold), the metastable intermediate structure, MIS (red), ferrite (blue) and cementite (green). Small dark spheres refer to C atoms. Dashed lines visualize the formed nano-twins during decomposition. The energy paths between the phases have been obtained by nudged elastic band calculations. Figure adapted from Ref. [18]*

the resulting time-temperature-transformation (TTT) diagrams, including the relation between the nose temperature for the fastest precipitate formation and the asymptotic temperature for the entropically-driven dissolution of all atoms in the matrix [10]. The fast determination of such trends would not have been possible without our Python based **workbench Pylron** discussed above. It is currently also used to identify fundamental rules for the solution of interstitial elements by analysing the results of high-throughput investigations (U. Aydin) and for running automated calculations with a prescribed error convergence (J. Jansen), which we consider as future challenge in the framework of integrated computational materials engineering (ICME).

The role of hydrogen for the stability of structural materials remained to be another important topic of the group that was triggered by various projects, primarily with industrial partners (see p. 39, see p. 163). In the last reporting period the investigations were focussed on a possible H enhanced decohesion of the interface between precipitates such as κ carbides (P. Dey), TiC (R. Nazarov) [33], and cementite (E. McEniry) [34] and the Fe matrix in steels. Further activities cover the interaction of H with vacancies (R. Nazarov) [19], chemical trends for the H solubility [35] and the understanding of the thermal desorption spectroscopy (E. McEniry).

Adaptive Structural Materials (B. Grabowski)

The general aim of the group is the design of advanced, next-generation structural materials based on innovative concepts driven by state-of-the-art simulation tools. To achieve this goal, also this group is focusing on further advancing the methods developed in the CM over the past years. These methods are rooted in accurate *ab initio* approaches and they extend to large scale molecular dynamics (MD) simulations based on empirical potentials and also to analytical approaches based on continuum theory. The group has a strong collaborative network within the MPIE (e.g., experimental ASM group in the MA) and with external partners from academia (e.g. Imperial College London or KTH Stockholm) and industry (Sandvik, Sweden). The projects investigated in the ASM group are ranging from simpler material systems, where the accuracy of the developed methods can be validated against experiment, to complex multiscale problems, where the focus is on understanding the atomistic mechanisms responsible for the experimental observations.

A core effort of the group is the development of efficient *ab initio* methods for highly accurate free energy determination at finite temperatures. This work is done in close collaboration with T. Hickel's group. A thermodynamic software package is being jointly developed that already allows to routinely employ previously developed methods such as the *upsampled thermodynamic integration using Langevin dynamics* (UP-TILD) method. We presently focus on computing phase stabilities of arbitrary structures, i.e. dynamically unstable solids, multicomponent systems, and liquids.

An important step in this direction has been recently taken with the introduction of the *two-stage upsampled thermodynamic integration using Langevin dynamics* (TU-TILD) method [36]. This development is based on a collaboration with A. Duff (former member of CM) and M. Finnis (Imperial College London), who are experts in the field of interatomic potentials. Combining their knowledge with our expertise in describing vibrational free energies, the TU-TILD

method was invented providing a large reduction in computational time (Fig. 6). The key idea is the introduction of an intermediate step based on optimized interatomic potentials. These potentials are fitted to *ab initio* MD trajectories at a specific volume and temperature. With this fitting procedure the transferability of the potentials is lost — a requirement in the usual construction of empirical potentials — but transferability is not needed for the TU-TILD method, since the potentials are only used as an optimized reference for thermodynamic integration. With this method we have enabled not only highly accurate and efficient calculations of the full vibrational spectrum, but also a very versatile approach allowing us to treat arbitrary structures.

Several projects within the ASM group are presently focused on exploiting the full power of the developed thermodynamic approaches: One of them is devoted to a highly accurate description of the temperature dependent phase stabilities in Ti (D. Korbmacher). This is a non-trivial task because the high temperature bcc phase is dynamically unstable and thus previously established rules fail to apply. A particularly important point is to understand the finite size constraints on the bcc to hexagonal (ω) phase transition, which we study with TU-TILD potentials. In another project, we further transfer and extend the knowledge gained for pure Ti to the binary Ni-Ti system (S. Maisel), which is technologically important its shape memory effect. The challenge in this project is to couple the vibrational excitations responsible for the stabilization of the dynamically unstable phases with the configurational entropy, which we tackle by integrating the cluster expansion method into our previous developments. Another exciting thermodynamic for development in the ASM group is the calculation of *ab initio* free energies of liquids (L. Zhu). The difficulty in determining the thermodynamics of liquids is that, in contrast to solid phases, no fixed lattice is available which could be used as a starting point. Our solution to this problem employs several intermediate thermodynamic integration steps between solid and liquid including also TU-TILD potentials.

Several collaborative projects broaden our spectrum of thermodynamic activities. A recently started project on temperature dependent stacking-fault-energies establishes a collaboration with R. Sahara (NIMS, Japan) who received a grant to stay for one year in our group. In another project we investigate the impact of lattice vibrations on local magnetic moments together with B. Alling (Linköping University, Sweden), who is presently a guest researcher under the Swedish International Career Grant. In a collaboration with A. Ready (Imperial College London) we apply our knowledge on bulk Ti and extend it to the description of defects (vacancies, impurity atoms, and their interactions), in order to understand the industrially relevant problem of low temperature

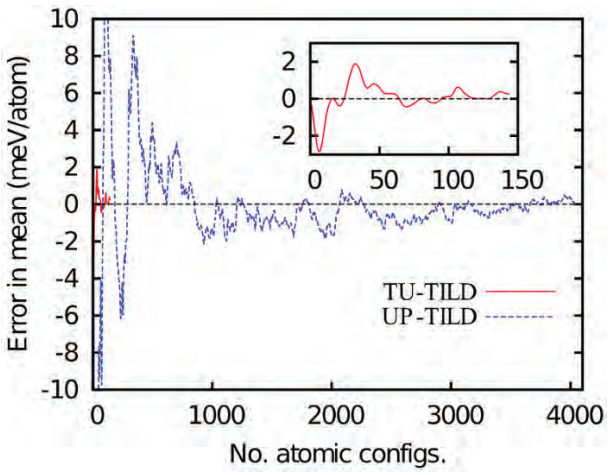

Fig. 6: *Example of the performance increase in computing ab initio free energies for ZrC by the newly developed TU-TILD method. Good statistical convergence can be now reached within a few hundreds of atomic configurations (red solid curve, inset) whereas several thousands of configurations were needed previously (blue dashed curve). Figure taken from Ref. [36].*

creep in Ti alloys. Another problem of industrial relevance is tackled in collaboration with B. Kaplan and A. Blomqvist (Sandvik, Sweden). The goal is to establish an accurate thermodynamic database for Cr carbides which are a critical component in tool steels.

The projects described so far are based on standard approximations to the exchange-correlation functional within density-functional theory (DFT). For a wide range of materials these approximations provide an excellent description of finite temperature properties up to the melting point. However, for some materials such as Au severe discrepancies are found in comparison to experiment. In collaboration with S. Wippermann from the GO, we have recently extended the UP-TILD method allowing now to compute finite temperature properties, in particular anharmonicity, at a level beyond the standard approximations [37]. Applying the new method to Au we could show that the severe discrepancies introduced by the standard functionals disappear (see p. 171).

In addition to the efforts relating to thermodynamic properties, projects are carried out where we apply and extend our finite temperature expertise to kinetic processes. One example is the investigation of grain boundary migration using large scale MD simulations (S. Hadian), which is essential to predict microstructure evolution and thereby the mechanical properties of materials. The present knowledge of grain boundary migration is limited and discrepancies between theory and experiment exist. We could recently show that, by overcoming the limits of state-of-the-art simulations and extending the simulations to fully 3D supercells and grain boundaries deviated from the symmetric case, new and unforeseen atomistic mechanisms occur, the

implications of which are presently investigated. This work on grain boundary migration is well embedded into the strategic plan of the MPIE (see p. 40) and cover figure of this report) and also well received by the experts in the community as became evident on the grain-boundary-migration conference we have recently organized (http://gb2015.mpie.de).

An important backbone of the ASM group is the close collaboration with the experimental ASM counterpart in the MA headed by C. Tasan. The joint efforts of the theoretical and experimental ASM groups are guided by the general strategy established in the SMARTMET ERC project (see p. 50), with the main idea of developing smart metallic materials. Specifically, we investigate mechanisms responsible for the unique properties of high entropy alloys (see p. 147) and we also intensively focus on phase transitions in Ti alloys. Recently, we started to apply our knowledge on Ti alloys to investigate routes for designing self-healing metals. This effort is embedded into the DFG priority programme SPP1568, which intends to advance self-healing in all material classes. In our project, we study whether shape-memory-alloy nano-particles can be applied as self-healing agents [38]. In particular, on the theory side, we are performing large scale MD simulations of the interaction of a nano-particle with a crack (W.-S. Ko). Our results are important guidelines for the corresponding experimental efforts of the self-healing project.

Beyond the projects mentioned so far, which are mainly focused on analysing a specific length scale by a suitable method, we investigate also complex material problems that require the application of multiscale approaches. As part of the department-wide research on hydrogen embrittlement, we have, for example, recently developed an atomistically informed analytic continuum approach allowing to predict nano-hydride formation in the strain field of dislocations (G. Leyson) [6]. This approach is accurate and efficient and allows therefore to compute complete phase diagrams (Fig. 7) which can be passed on to higher level approaches like discrete dislocation dynamics or finite element analysis. This is an important step towards quantifying the effect of hydrogen localization around dislocations to fracture mechanisms. In another multiscale project, the mechanisms causing C supersaturation of the ferrite phase in a severely drawn pearlitic wire are investigated (A. Nematollahi). Such wires are the world record holders having the highest tensile strengths in structural materials with up to 7 GPa. The mechanisms causing these special properties are not yet fully understood, but atom probe tomography performed in the MA suggests that cementite decomposition and the resulting C supersaturation of ferrite is a decisive factor. A. Nematollahi has recently successfully finished his PhD thesis on this topic, where he employed different methods on various length scales showing that dislocations are the main source of the supersaturation. In addition to the thermodynamic stabilization of C around dislocations, he could show by atomistic barrier calculations and by solving a corresponding diffusion equation that there is a realistic drag mechanism which could lead to the observed cementite decomposition. These theoretical results nicely support and explain the complementary experimental observations performed in the MA and SN (see p. 183).

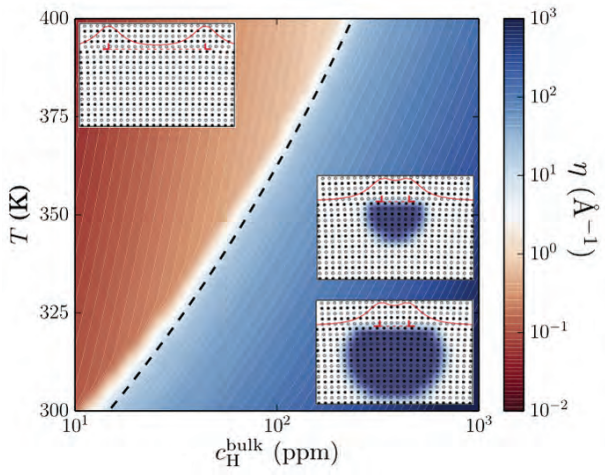

Fig. 7: *Example of a nano hydride phase diagram around an edge dislocation in fcc Ni as a function of bulk hydrogen concentration c_H^{bulk} and temperature T. The colour indicates the excess hydrogen, η,, per unit length of the dislocation. In the blue part of the phase diagram a nano-hydride is formed, whereas it is destroyed by configurational entropy in the red part. The three insets show a region around the dislocation core (indicated by the red lines) without and with nano-hydride (highlighted by the blue colour).*

Mesoscale Simulations (R. Spatschek; until October 1, 2015)

The research in this group is devoted to the understanding of **scale bridging phenomena appearing on dimensions between the atomic and continuum scales**. Various computational and analytical techniques, which are particularly tailored to the different applications, are used in this group. The further development and improvement of models and simulation techniques is also an important activity. In the following, recent key activities are briefly discussed.

The understanding of **hydrogen embrittlement** is a central topic for the group and linked to the SFB 761 (see p. 52). Together with T. Hickel's group, the site preference of hydrogen atoms in Fe-Mn alloys has been investigated. It turns out that H prefers a Mn-rich environment, which to a large extend can be attributed to volumetric effects [35]. Such ab initio information is further passed to continuum descrip-

tions of coherent hydride formation in the bulk and near surfaces. We found that the hydrogen solubility limit near free surfaces is significantly lower due to elastic relaxation, which enhances the nucleation of detrimental brittle hydrides in these regions and at cracks (G. Gobbi, C. Hüter).

Within the DFG priority programme SPP1713 we investigate **bainite formation in partial press hardening processes** as a joint project between the MPIE Düsseldorf, RWTH Aachen University and IWT Bremen. Press hardening, also known as hot stamping, has become an important processing technology for the production of high strength steels mainly for automotive industry. Conventionally, the underlying concept is the rapid quenching of the austenite to the martensite state. Recent developments use interrupted cooling plus quasi isothermal holding in the bainite region, yielding partly bainitic structures with very attractive properties. This technique is called bainitic press hardening and it offers advanced strength-failure-strain combinations. We pursue a scale bridging description of the phase transformation kinetics during the forming process, which starts from fundamental microscopic properties and goes up to effective descriptions on macroscopic scales [39] (C. Hüter).

The thermodynamics and kinetics of **grain boundaries** has been investigated by means of amplitude equations approaches, which supplement conventional phase field models by preserving atomic resolution. The appearance of temperature dependent dislocation pairing transitions in symmetric tilt grain boundaries is found to be in agreement with predictions from atomistic simulations and phase field crystal simulations [40]. Shear coupled motion of grain boundaries is found to obey the geometrical model of Cahn and Taylor, including also grain rotation [41]. The methodology has also been applied to extended defects in nanowires, including scaling predictions for the growth conditions of coherent nanowires [42, 43] (C. Hüter, G. Boussinot, C.-D. Nguyen).

As a continuation of our activities on **grain boundary melting** we transferred our findings on short ranged interactions between adjacent grains to larger scales [44, 45]. These short range forces locally modify the thermodynamics on the nanometre scale and can induce grain boundary premelting of high angle grain boundaries below the bulk melting point. To understand the implications of these effects for the kinetics of melting processes along grain boundaries, we combined them with mesoscale concepts for microstructure evolution modelling. It turns out that the microscopic effects indeed can have a significant influence on the steady state velocity of the mesoscopic front propagation (Fig. 8) [46]. Whereas the used sharp interface approaches are particularly

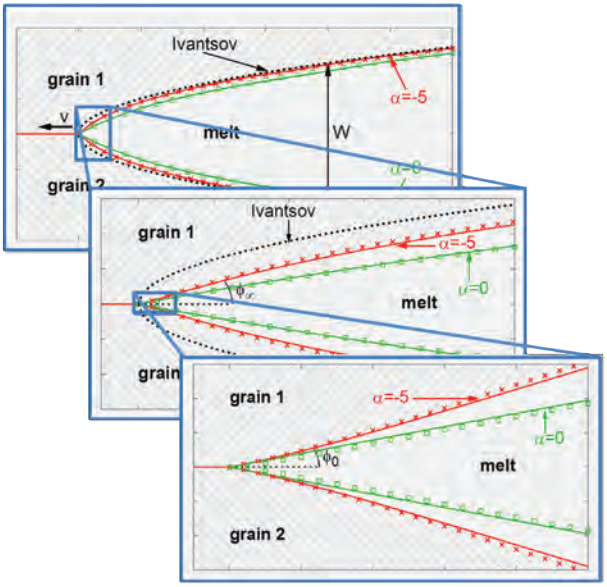

Fig. 8: *Hierarchy of scales for the melting along overheated grain boundaries. On the mesoscale (background) the melt front has a parabolic front. At the tip (magnified), a finite mesoscopic dihedral angle forms. On the nanometre scale (front panel) the solid-melt interfaces are not straight due to the mutual short ranged interaction between nearby solid-melt interfaces. α is a dimensionless measure for the strength of the short range interaction [46].*

useful for a closed analytical understanding of the dependence on material parameters, actual simulations of grain boundary melting in polycrystalline materials are easier to perform using phase field methods. For that, we have investigated how the short ranged interactions are related to the intrinsic phase field model parameters for a quantitative mapping between the different methods [47]. A comparison between the predicted melting velocities from the sharp interface and phase field methods provides the tools for large scale simulations [48] (P. Bhogireddy, F. Twiste, C. Hüter).

Peritectic phase diagrams are essential for many alloys and in particular for steels. We have studied different growth morphologies during **peritectic solidification**. We have investigated dendritic growth as a result of the peritectic reaction, and have compared this case to coupled cellular growth. The latter is of practical interest for the formation of composite materials directly during casting, as for example in Fe-Ni alloys. We find that depending on the spacing of the primary solidification, a morphological transition between dendritic and cellular growth occurs [49] (G. Boussinot, C. Hüter).

A new activity, which has been launched during the past years, is the modelling of **frictional phe-**

nomena (Fig. 9). Starting point is the well-known fact that the dynamic friction coefficient is typically velocity-dependent. The usual believe is that it is decaying with increasing velocity, as a result of the reduced time for micro-contact ageing. However, we have pointed out in an extended survey that many materials indeed show such a velocity weakening behaviour only at moderately low sliding speeds, whereas often a transition to a velocity strengthening regime at higher velocities, where the friction coefficient increases with speed, is rather the rule than the exception [50]. The appearance of a minimum frictional force in the transition regime has tremendous consequences for rupture fronts, which are travelling along a bi-material interface. In contrast to conventional "earthquake-like" events, which propagate essentially with the speed of sound, so called "slow fronts" with significantly lower velocities can emerge near the minimum of the frictional force [51]. Creep patches, which are a localized weakening of the micro-contacts at the interface under shear, often appear as precursors to these slow fronts, in agreement with recent laboratory observations of such periodic events [52]. Whereas the appearance of frictional instabilities on all scales from atomistic to geological dimensions is often attributed to a velocity-weakening behaviour, we recently found that also on the strengthening branch instabilities can occur for a strong bi-material contrast. The major difference between the two cases is that the latter is related to high frequency elastodynamic effects. The behaviour is expressed in terms of universal stability diagrams for large sample heights. In contrast, for thin samples (relative to the wavelength of the instability) waveguide-like modes can emerge, which are universally unstable [53] (M. Weikamp, R. Spatschek).

Several efforts have been made for the **development of phase field models** for mesoscale microstructure evolution modelling. The long-standing problem of thermodynamic consistency for phase field models with a thin interface limit for superior convergence behaviour has been solved. Here the antitrapping current prevents artificial solute segregation in the presence of a diffusional contrast between phases. It turns out, that a consistent model, which obeys the Onsager symmetries, also has to take into account proper off-diagonal cross couplings between concentration and phase fields for achieving realistic kinetics and to satisfy all boundary conditions. This also allows the elimination of spurious surface diffusion effects and temperature discontinuities at the interface (Kapitza jump) [54,-56]. Plastic effects and phase transformations induced by Joule heating by an external electrical field are considered in [57, 58], and additionally resulted in efficient implementations of the codes on graphics cards, which can accelerate the code by up to two orders of magnitude in comparison to a conventional CPU code (G. Boussinot, C. Hüter).

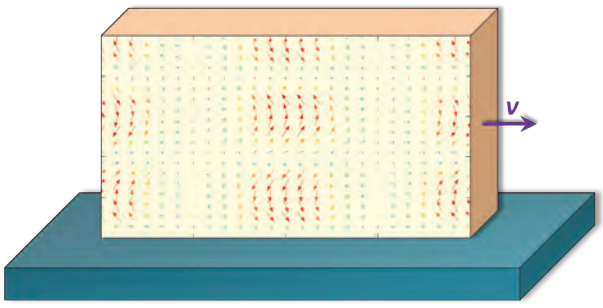

Fig. 9: *Frictional sliding on a rigid substrate with velocity v. For a thin slider waveguide like modes can form inside the slider and trigger a high frequency instability [53]. The displacement field of the standing waves is illustrated by the arrows.*

Defect Chemistry and Spectroscopy (C. Freysoldt)

This group focuses on atomic-scale defects in non-metallic materials such as oxides, electrolytes, or semiconductors by means of *ab initio* methods, and develops state-of-the-art methods and concepts for this purpose.

Point defects exert a critical influence on the electrical, chemical, transport, and other properties of real oxides and insulating materials. Computer simulations are a powerful tool to better understand the formation of point defects, their properties, and their role in modifying macroscopic material parameters [11]. Major challenges in the simulation arise from (1) providing a reliable theoretical framework to accurately compute the defect energetics, notably the formation energy and electrically active transitions within the band gap of the material, (2) from linking the microscopic picture to a coarse-grained theory that is able to describe the experimentally relevant time and length-scale (scale bridging), and (3) from developing useful approaches for point defects in alloys or amorphous materials.

The development of the **multi-scale programme package SPHInX** (available at http://sxlib.mpie.de) is a continuous activity of the group. A highlight from the past period is the extension of the MPI parallelization to automatic multi-loop parallelization in collaboration with the Max Planck Society Computing Centre in Garching and the exploration of optimizing the performance by hardware-specific (GPU = Graphic Processor Unit, AVX = Advanced Vector Extensions) algorithms for key functions. Further external collaborators on SPHInX development are S. Boeck (Gemmantics IT Consulting, Erkrath) and O. Marquardt (Paul-Drude-Institut, Berlin). Recent in-house developments cover the robust implementation of atomic-spin constraints (M. Grabowski) and

a correction scheme for electrostatic interactions between defects at surfaces and interfaces.

Group III nitrides for optoelectronic device applications. To better understand the properties and growth of ternary nitride alloys, we study local ordering phenomena in epitaxially strained $In_xGa_{1-x}N$ layers and the associated finite-temperature thermodynamics by means of Monte-Carlo simulations (S. Lee). Our calculations predict the existence of a hitherto unknown ordered phase at 33% In composition [59]. An important problem for optoelectronic devices is the identification of loss mechanisms. The group has therefore worked on identifying which point defects may act as centres for non-radiative recombination (Y. Cui). Moreover, we worked on understanding the composition dependence of elastic and electronic properties of $In_xGa_{1-x}N$ layers grown on GaN [60, 61], as well as understanding the growth of GaN on Ge(111) as an alternative substrate [62] (Y. Cui) (Fig. 10). The methods developed here can be directly transferred to understand and predict orientation relationships of coherent precipitates or inclusions in structural materials such as steels.

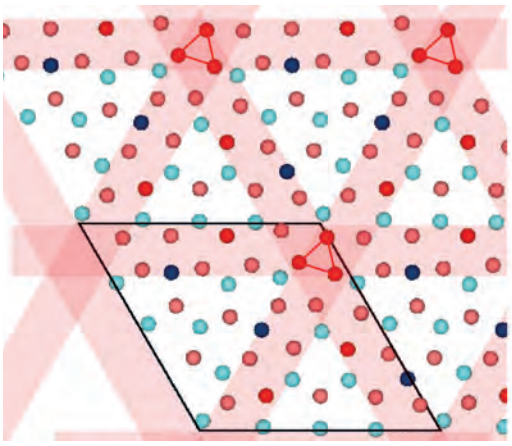

Fig. 10: *Calculated interface structure of a semicoherent Ge(111)/GaN(0001) interface with a 4:5 lattice match. Shown are the topmost Ge layers that translate the lattice match from 4 rows (Ge), in blue, to 5 rows (GaN), in red. The insertion of the extra rows (shaded stripes) are adopted by rebonding the tetrahedrally coordinated Ge atoms, leading to a small number of 5-fold coordinated Ge atoms. The model predicts interlayer separations in good agreement with experiment [62].*

A further area of interest has been to understand the role of **electrostatics** for atomic-scale simulations **at surfaces**, both for adsorbate-adsorbate interactions at metallic surfaces in collaboration with the group of M. Todorova [7], but also for charged defects at surfaces and interfaces, generalizing the Freysoldt-Neugebauer-van-de-Walle correction scheme for bulk defects to such systems.

Electrochemistry and Corrosion (M. Todorova)

The group aims to develop *ab-initio* based multiscale simulation techniques and apply them to problems in electrochemistry, with a strong focus on corrosion and related topics. The various activities in the group are tailored to provide in-depth insight into the functionality and evolvement of materials properties under the influence of the environment. Such insight will aid the **development of strategies to counteract, retard or suppress degradation phenomena in materials** (see p. 28).

As a first-step in this direction we have developed a unified approach that is based on a fully grand-canonical description of both ions and electrons and that connects and “translates” concepts in semiconductor defect chemistry and electrochemistry [63]. Our method links *ab initio* calculations quite naturally to experimental observables, such as the pH-scale and the electrode potential, which determine and characterise the state of an electrochemical system. It provides surprising new insight into apparently ”old” problems such as water stability, opens new routes to construct electrochemical phase (Pourbaix) diagrams and gives a handle to an absolute alignment of electrochemical potentials. The microscopic understanding gained makes it, furthermore, possible to obtain ion hydration/solvation energies by a hitherto not explored route. The developed approach provides a firm footing to the activities in the group, which are tailored to facilitate knowledge about the elementary process, important in the context of wet-electrochemistry, their interplay and specific corrosion related questions.

The **interactions of atoms and molecules with surfaces** are at the onset of materials’ degradation mechanisms, such as **corrosion in reactive environments**. The investigation of the oxidation behaviour of Mg and Mg/Zn alloys by means of density functional theory calculations, is one example of research in this area (S.-T. Cheng). An interesting outcome is the high propensity of Mg to oxidise. Usually the adsorption of electronegative elements on metal surfaces leads to an increase in work function and a decrease in binding energy as the adsorbate coverage rises. A decrease in work-function and an increase in binding energy, i.e. the opposite behaviour, is observed for N, O and F on Mg(0001). Analyses of the electronic structure shows that this unusual adsorption behaviour is a consequence of a highly polarisable electron spill-out present in front of the Mg(0001) surface, which is responsible for the appearance of a hitherto unknown net-attractive lateral electrostatic interaction between same charged adsorbates (Fig. 11). Understanding this novel type of bonding allows us to rationalise the high propen-

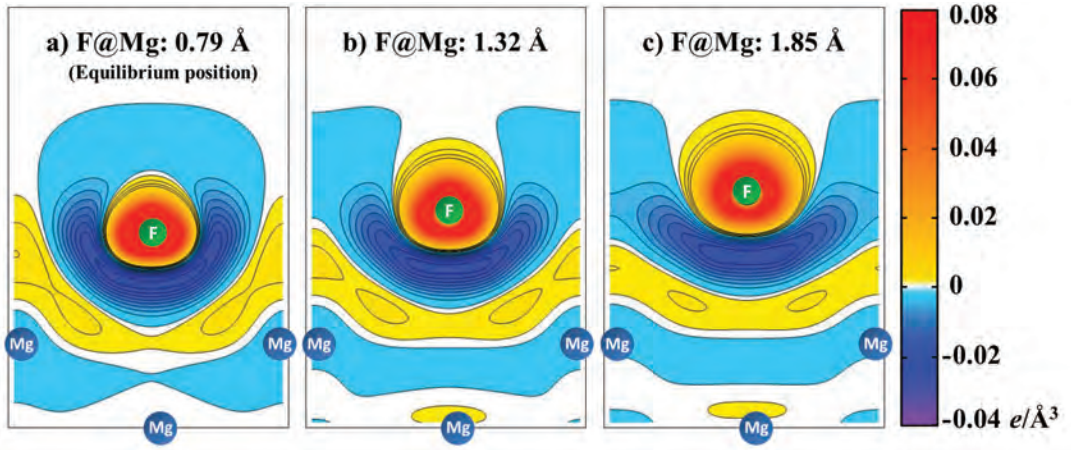

Fig. 11: *Difference electron density plots for 0.25 mono-layers of F adsorbed at different heights above the Mg(0001) surface. It visualizes the efficient embedding of F at its equilibrium adsorption position within the spill-out electron region of the surface, which facilitates the attractive interaction between the same charged adsorbates.*

sity of magnesium to corrode and get insight into the initial stages of corrosion - the arising attractive interactions lead to a spatial localisation of reactive atoms, which results in an earlier onset of oxidation at a given adsorbate's chemical potential [7].

Another example investigating the interactions of H_2S with Fe-surfaces (M. Ilhan) in the context of sour-gas corrosion is highlighted in p. 165.

An important step towards the modelling of, e.g., **metal dissolution or wet corrosion** is the ability to accurately describe ions and their solvation shells at the solid/liquid interface, within its proximity and within the bulk solution of an electrolyte. Studying ions near the interface requires including electric fields, the interaction with a (charged) surface, possible ion or field induced surface reconstructions. A realistic description of these phenomena and their interplay requires substantial new method developments which are underway or will be addressed in forthcoming investigations. The case of ions in bulk electrolyte is seemingly "easier" to tackle and provides one advantage – it allows us to gauge and develop our methodology by comparing calculated quantities to measurable observables. In this context systematic studies performed by A. Vatti present an important milestone. His investigations on the influence of various parameters (e.g. temperature, pressure, water surface dipole, DFT-functional) on the formation energies of ions in water allow us to access the importance of different contributions and to develop a protocol to calculated accurate ion formation energies (Fig. 12). It, furthermore, enables us to consolidate the approach usually used within the chemical/biological community, in which an ion in vacuum is considered the reference state for ion solvation, and the semiconductor based approach employed by us, in which the elemental state of the atom is considered the reference. A comparison of the calculated formation energies and transition levels for the investigated ions Cl, I, Br and Zn ions are found to accurately reproduce the experimental values. Hereby methodologies, such as the Freysoldt-Neugebauer-van-de-Walle correction scheme, developed for charged defects in semiconductors are of central importance.

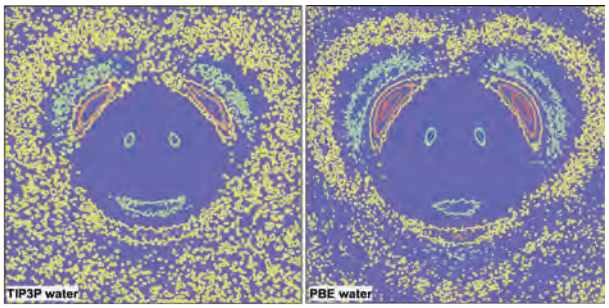

Fig. 12: *2D radial distribution function of water, which visualizes density variations as a function of distance from a chosen oxygen atom, obtained by molecular dynamic simulations with the popular classical potential (TIP3P) and the PBE exchange-correlation functional, which is known to overstructure water.*

A process which can be either utilised (i.e. to enhance the speed of drilling) or presents severe problems (i.e. cause major incidents in industrial plants) in industrial applications is **liquid metal embrittlement**. The liquid metal embrittlement of Fe by Zn [64] was studied in collaboration with K.-D. Bauer and K. Hingerl (Linz University, Austria). Evaluating the difference between the DFT-calculated grain boundary and the surface energies of the corresponding surfaces by utilising both the canonical Griffith and the grand-canonical Wang-Rice model showed that the Zn induced weakening of the GB sets in in the Wang-Rice formulation for Zn concentrations which are 2-3 orders of magnitude lower than in the Griffith case. Since the Wang-Rice model assumes suffi-

ciently mobile Zn, which is able to preserve a constant Zn chemical potential at the crack tip as the crack propagates, and the canonical model assumes that the Zn amount present within the GB is preserved at the surface, i.e. it remains unchanged, this suggests that kinetic barriers in Zn diffusion can largely reduce the undesired effect of GB weakening. The attempt to combine the insights obtained from DFT based modelling with the continuum models employed and developed in the group of R. Spatschek is the topic of an ongoing project of the MPIE doctoral programme SurMat (P. Bhogireddy).

Further activities in the group focus on the stability of surfaces, interfaces or materials under the influence of the environment. The **identification of stable and metastable surface/interface structure subject to the given environmental conditions** is aided by the construction of surface Pourbaix diagrams. One example is our continuing work on the stability on polar ZnO(0001)-Zn surfaces, in which we focus on the interface phases in an aqueous electrolyte (S. Yoo). These provide the basis for comparison to experimental measurements performed in the groups of M. Valtiner (GO) and K. Morgenstern (Ruhr University Bochum). A further example are the **investigations of materials stability, understanding of stabilisation/destabilisation mechanisms and oxide growth** related to the construction of defect-phase diagrams [65, 5]. Such diagrams identify the majority defect species as functions of applied bias and chemical potential and allow discussions about the impact that aqueous electrolyte has on the electronic structure of a semiconducting electrode, thus providing insight into areas of interest in the context of electrochemical applications, such as corrosion. (see p. 161).

Growth Modelling (L. Lymperakis)

The focus of the growth modelling project group is on the epitaxial growth of compound semiconductors with a strong focus on III-Nitride materials. The topics of interest include the thermodynamics and kinetics of epitaxial growth [8, 66, 67], the electronic properties of surfaces [68, 69] and extended defects [70], as well as the growth and optoelectronic properties of semiconductor nanostructures [71]. Within the reported period L. Lymperakis was and is active in three EU funded projects: (i) The Industry-Academia Marie-Curie project SINOPLE, (ii) the Nanosciences, Nanotechnologies, Materials and new Production Technologies project ALIGHT, and (iii) ECSEL Joined Undertaking project PowerBase. Selected topics that were and are addressed in this area are:

The **growth of high In content InGaN alloys** with sufficiently high crystal quality constitutes a puzzling situation where the complex interplay between surface morphologies, partial pressures and growth temperature plays a central role. We have investigated the bulk and surface thermodynamics of $In_xGa_{1-x}N$ growth for the technologically relevant (0001) and (0 0 0 $\bar{1}$) growth planes by means of DFT calculations. Our calculations reveal that chemical effects (i.e. stronger Ga-N as compared to In-N bonds) result in a strong driving force for In surface segregation in the (0001) growth [8]. Furthermore, the thermal stability of excess In is found to be remarkably higher on N-polar surfaces than on the Ga-polar surfaces, indicating that for a given level of In incorporation, higher temperatures can be used for N-polar growth as compared to Ga-polar growth [67]. We have furthermore investigated the thermodynamics of solid and gas phases in molecular beam epitaxy like growth conditions and we highlighted the effect that plasma discharges have on the critical temperatures for InGaN decomposition: The weaker binding of the active nitrogen species produced by plasma as compared to ground state molecular nitrogen shifts the equilibrium and thus the maximum allowed growth temperatures to ≈500K higher values. However, the aforementioned temperatures have to be decreased by ≈100K for every 25% InN added to the InGaN alloy (A. Duff).

Surfactants and antisurfactants are species, deposited prior to growth on the substrate to overcome fundamental limitations set by thermodynamics and adatom kinetics in a particular heteroepitaxial system. The role and mechanisms of surfactants and self-surfactants in the growth of group III-Nitrides is well established and understood. However, the physics governing the technological important example of Si as antisurfactant in GaN was under intensive debate. In contrast to surfactants that mainly modify the growth mode by influencing adatom kinetics, we have revealed that antisurfactants modify the chemical potentials at the surface. This is based on the formation of a single $SiGaN_3$ subsurface monolayer (Fig. 13) that is **electrically active** and introduces a dipole moment caused by a charge transfer from the aforementioned layer to the surface [66]. Hence, growth proceeds in a lateral epitaxial overgrowth way only at locations where the $SiGaN_3$ layer is not present and allows to block and reduce the density of threading dislocations (in cooperation with M. Albrecht, Leibniz Institute for Crystal Growth, Berlin). Dislocations are extended defects that induce electronic states into the bandgap of semiconductors. However, a particularly interesting case is the **perfect screw dislocations** in a direct band gap semiconductor: The core of the defect consists of fully coordinated atoms and exhibits in first order a pure shear strain field. Thus, apart from their technological importance, these defects allow to investigate the physics underlying the effect of **shear strains on the electronic structure of semiconductors**. In order to investigate the later we developed an ***ab-initio* based**

quasi-continuum approach which combines DFT calculations with elasticity theory and we investigated the electronic properties of *a*-type screw dislocations in GaN [70]. In contrast to the common picture of exciton localization by screw dislocations, our analysis revealed that both the valence band maximum as well as the *s*-type, and hence in principle insensitive to shear strains, conduction band minimum (CBM) bend into the bandgap. This unexpected and with previous concepts not understandable downward shift of the CBM was shown to be a consequence of higher lying conduction bands that have *p* character and that are due to the huge strain fields around screw dislocations in GaN so strongly shifted that they hybridize with the band edge (in cooperation with M. Albrecht, Leibniz Institute for Crystal Growth, Berlin).

Wulff diagrams constitute a powerful tool to understand and control homo- and hetero-epitaxy along various crystallographic orientations and can be used to predict and design the growth of thermodynamically stable surface morphologies. However, due to the low point-group symmetry of the wurtzite crystal structure, polar and semipolar surface energies of these crystals are ill defined. Nevertheless, by invoking the similarities between the wurtzite {0001} and zincblende {111} planes, surface energies of the former can be calculated. Our calculations revealed that under typical GaN MBE (molecular beam epitaxy) growth conditions, the surface energies are independent of surface orientation and the mechanism to minimize the surface energy is to minimize the surface area. However, for the industry preferred HVPE (hydride vapour phase epitaxy) and MOCVD (metal organic chemical vapor deposition) growth, the surface energies show a strong orientation dependence having deep cusps at the polar (0001), non-polar (1 1 $\bar{2}$ 0) and the semipolar (1 1 $\bar{2}$ 2) orientation. This indicates that other semipolar (1 1 $\bar{2}$ /) orientations under conditions of thermodynamic equilibrium are prone to roughening and/or faceting towards the aforementioned planes.In a PhD project that started in January 2015 the **electronic properties and thermodynamics of point defects in oxide- and organometallic- perovskites** are investigated. $SrTiO_3$ constitutes a representative model for the wide class of large bandgap perovskites and has attracted considerable attention due to the two-dimensional electron gas (2DEG) observed at the interface with $LaAlO_3$ as well as due to the strong photocatalytic property under ultraviolet light. Halide perovskites are under an unprecedented progress thanks to their remarkably high efficiency in solar cell applications. In the first period the focus of the project is on the thermodynamics and electronic properties of oxygen single and di-vacancies in $SrTiO_3$ which are investigated by means of hybrid functional calculations. In the second period the focus will shift to inorganic-organic hybrid perovskite materials (M. Alam, in collaboration with MA and SN).

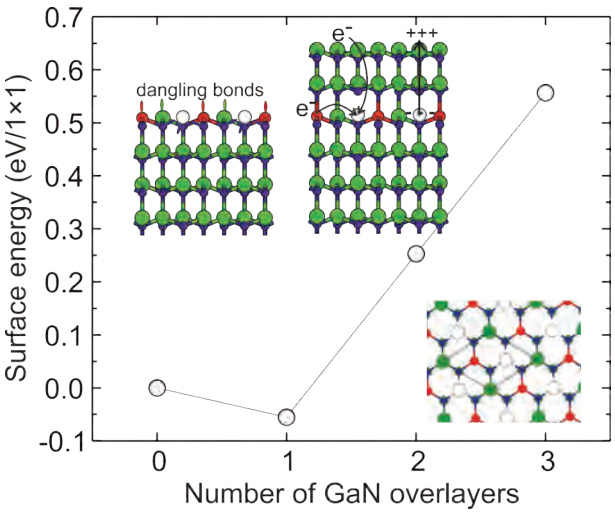

Fig. 13: *Surface energies, referenced with respect to the $SiGaN_3$ terminated surface, as function of the number of GaN overlayers grown above the $SiGaN_3$ layer. The upper insets represent the atomic configurations without and with two GaN overlayers, respectively. In the case of 2 GaN overlayers the charge transfer and the build in electrical dipole moment are indicated. The bottom inset represents a top view of the $SiGaN_3$ layer. The dashed frame indicates the $\sqrt{3}\times\sqrt{3}R30^o$ construction. Green, blue, red, and white balls indicate Ga, N, Si atoms and Ga vacancies, respectively. Figure taken from Ref. [66].*

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Research Projects in Progress

Computational Phase Studies

Aydin, Hickel, Neugebauer: Chemical trends for the solubility of interstitials in metals using high-throughput calculations and machine learning

Begum, Dutta, Hickel: Monte-Carlo simulations of magnetic model Hamiltonians

Bleskov, Hickel, Neugebauer, Raabe (in collaboration with R. Dronskowski, B. Hallstedt et al., RWTH Aachen): Ab initio calculation of free energies, stacking-fault and grain-boundary energies at finite temperatures in Fe-Mn-C alloys

Dey, Hickel (in collaboration with Z. Georgeou, F. Klose, Salzgitter Mannesmann Forschung GmbH): Impact of microstructure on hydrogen embrittlement in Cr-containing high-Mn steels

Dey, Hickel (in collaboration with B. Gehrmann, J. Klöwer, VDM Metals GmbH, Research & Development): Ab initio study on the interaction of hydrogen and microstructure in the alloys system 718

Dutta, Hickel (in collaboration with A. Hütten, A. Waske** (*Universität Bielefeld, **IFW Dresden)):* Coupling phenomena in magnetocaloric materials: From thin layers to composites

Dutta, Hickel (in collaboration with S. Ghosh, B. Sanyal** (*IIT Guwahati, India, **Uppsala University, Sweden)): Ab initio* study of lattice dynamics in systems with magnetic disorder

Glensk, Grabowski, Hickel, Neugebauer (in collaboration with B. Hallstedt, I. Egry**, R. Schmid-Fetzer***, M. Rettenmayr**** (*RWTH Aachen, **DLR Köln,***TU Clausthal, ****U Jena)): Ab initio* determination of Helmholtz free energies and derived properties (phase diagrams, heat capacities, thermal expansions) for Al alloys containing Si, Mg and Cu

Glensk, Grabowski, Hickel, Neugebauer: Anharmonic contributions to *ab initio* computed thermodynamic material properties

Glensk, Grabowski, Hickel, Neugebauer (in collaboration with P. Neibecker and M. Leitner, Technische Universität München): Accurate determination of phonon linewidths

Gupta, Dutta, Hickel (in collaboration with S. Divinski, G. Wilde, Universität Münster): Mechano-chemical coupling during precipitate formation in Al-based alloys

Janßen, Hickel, Neugebauer: Automatized determination of error bars of *ab initio* derived quantities using the PyIron workbench

Janßen, Hickel, Neugebauer (in collaboration with C.C.Fu, F. Soisson*, H. Amara**, V. Pierron-Bohnes***, S. Divinski****, R. Drautz***** (*CEA Saclay, France, **LEM, France,***IPCMS Strasbourg, France, ****Uni Münster, *****Ruhr-Universität Bochum)):* Magnetism in iron alloys: thermodynamics, kinetics and defects

Körmann, Hickel, Neugebauer (in collaboration with M. Staadt, J. Rogal*, R. Drautz* (*ICAMS, Bochum)): Ab initio* simulation of magnetic contributions to the thermodynamics of metals

McEniry, Hickel (in collaboration with S. Merzlikin, T. Schablitzki**, J. Rogal**, R. Drautz**, O. Rott***, T. Pretorius*** (*GO department, **Ruhr university Bochum, **ThyssenKrupp Steel Europe AG)):* Experimental and atomistic analysis of thermal desorption spectroscopy (TDS) in steels

Sözen, Hickel (in collaboration with Y. Ouyang (*Guangxi University, China)):* Mechanisms of self and impurity diffusion in Fe-Al intermetallic compounds

Sözen, Hickel, Neugebauer (in collaboration with L. Kunz, T. Eckl*, C. Elsässer* (*Robert Bosch GmbH, Applied Research, **Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg)): Ab initio* simulation of hard-magnetic materials

Zendegani, Körmann, Hickel (in collaboration with A. Ladines T. Hammerschmidt, R. Drautz (Ruhr-Universität Bochum)): Ab initio based calculation of the stability of selected TCP precipitates in steels: Temperature and interface effects

Zendegani, Körmann, Hickel, Neugebauer (in collaboration with B. Hallstedt, R. Schmid-Fetzer***, M. Rettenmayr*** (*RWTH Aachen, **TU Clausthal, ***U Jena)):* First-principles study of thermodynamic properties of the Q-phase in Al-Cu-Mg-Si

Zhang, Hickel, Neugebauer (in collaboration with J. Rogal and R. Drautz, Ruhr-Universität Bochum): Structural transformations in Fe-C alloys: From atomistic simulations to a microscopic understanding

Adaptive Structural Materials

Korbmacher, Grabowski, Neugebauer: Highly accurate description of temperature driven phase transitions in Ti-alloys

Zhu, Grabowski, Neugebauer: *Ab initio* description of free energies of liquids

Maisel, Grabowski, Neugebauer: Coupling of vibrational free energies with the cluster expansion technique

Hadian, Grabowski, Neugebauer (in collaboration with C. Race, University of Manchester): Molecular dynamics simulations of grain boundary migration

Leyson, Grabowski, Neugebauer: Multiscale modeling of hydrogen enhanced homogeneous dislocation nucleation

Nematollahi, Grabowski, Neugebauer (in collaboration with Y. Li, MA department and S. Djaziri, SN department): Atomic scale analysis of the origin of pearlite‘s strength

Ko, Grabowski, Neugebauer (in collaboration J. Behler, Ruhr-Universität Bochum): Development of neural-network potentials for NiTi

Sahara, Grabowski, Neugebauer: Temperature dependent stacking-fault-energies in Co from *ab initio*

Alling, Grabowski, Glensk, Neugebauer (in collaboration F. Körmann, TU Delft and I. Abrikosov, Linköping University): Impact of lattice vibrations on electronic and magnetic properties of paramagnetic Fe

Glensk, Grabowski, Hickel, Neugebauer (in collaboration with P. Neibecker and M. Leitner, Technische Universität München): Accurate determination of phonon linewidths

Korbmacher, Grabowski, Neugebauer (in collaboration with A. Duff and M. Finnis, Imperial College London): Development of the TU-TILD method

Grabowski, Neugebauer (in collaboration with C. Tasan and D. Raabe, MA department): SMARTMET: Adaptive nanostructures in next generation metallic materials

Grabowski, Neugebauer (in collaboration with D. Ma, MA department and F. Körmann, TU Delft): Phase stabilities in high entropy alloys

Grabowski, Hickel, Neugebauer (in collaboration with F. Körmann, TU Delft, R. Reed, University of Birmingham, and A. Ruban, KTH Stockholm): Temperature dependent stacking-fault-energies in Al, Cu, and Ni from *ab initio*

Grabowski, Neugebauer (in collaboration with A. Ready and A. Sutton, Imperial College London): *Ab initio* description of point defects in Ti

Grabowski, Neugebauer (in collaboration with L. Huber, M. Militzer, J. Rottler, University of British Columbia, Vancouver): Concurrent QM/MM coupling in metals

Grabowski, Ko (in collaboration with C. Tasan, MA department): Self-healing metals

Grabowski, Korbmacher (in collaboration with B. Kaplan, KTH Stockholm and A. Blomqvist, Sandvik Company): Finite temperature **ab initio** calculated thermodynamic properties of orthorhombic Cr3C2

Grabowski (in collaboration with S. Bigdeli and M. Selleby, KTH Stockholm): *Ab initio* description of phase stabilities in Mn

Mesoscale Simulations

Spatschek, Neugebauer: Ab initio based mesoscale description of hydrogen embrittlement

Spatschek (in collaboration with A. Karma, and I. Steinbach**; *Northeastern University Boston, **Ruhr-Universität Bochum):* Grain boundary premelting

Spatschek (in collaboration with E.A. Brener, E. Bouchbinder**, *Forschungszentrum Jülich, **Weizmann Institute of Science, Rehovot, Israel):* Instabilities during frictional sliding

Spatschek (in collaboration with I. Steinbach, Ruhr-Universität Bochum): Liquid metal embrittlement

Spatschek (in collaboration with A. Monas, M. Apel**, E.A. Brener***, *ICAMS, Ruhr-Universität Bochum, **ACCESS Aachen, ***Forschungszentrum Jülich)*: Phase transformations with Joule heating

Spatschek (in collaboration with B. Eidel, Universität Siegen): Plastic effects on the kinetics of phase transformations

Spatschek (in collaboration with U. Prahl, M. Hunkel**, *IEHK, RWTH Aachen, **IWT Bremen):* Bainitic press hardening

Spatschek (in collaboration with G. Boussinot, E.A. Brener**, *ACCESS Aachen, **Research Center Jülich):* Peritectic solidification

Spatschek (in collaboration with M. Friák, Brno, Czech republic): Nonlinear elasticity

Spatschek (in collaboration with M. Finnis, Imperial College London): Phase field modeling of oxide scale growth

Defect Chemistry and Spectroscopy

M. Grabowski, Freysoldt, Neugebauer: Atomic spin constraints in density functional theory

Koprek, Freysoldt, Neugebauer: Element distribution at CdS/CIGS interfaces in solar cells

Freysoldt, Neugebauer (in collaboration with S. Zhang, University of Cambridge): Electronic properties of InGaN under finite strains

Freysoldt (in collaboration with K. Reuter, Garching Computing Center, Germany): Parallel algorithms for atomic orbital projections from plane-wave basis sets

Freysoldt, Neugebauer (in collaboration with C. Liebscher, SN): Electron spectroscopy of CuCr

Freysoldt, Neugebauer: Phonons in ionic systems

Electrochemistry and Corrosion Science

Cheng, Todorova, Friák, Neugebauer (in collaboration with M. Rohwerder, GO department): A density functional theory study on the oxidation behaviour of Mg and Mg-Zn alloys

Vatti, Todorova, Neugebauer (in collaboration with M. Valtiner, GO department): Direct experimental measurements and theoretical *ab initio* simulations of hydration layers and specific ion adsorption at confined solid/water/solid interfaces

Yoo, Todorova, Neugebauer (in collaboration with M. Valtiner, GO department and K. Morgenstern, RUB): Stability of electrode materials in an electrochemical environment

Surendralal, Todorova, Neugebauer: Machine-aided calculations of charged point defects in magnesium and iron oxides

Todorova, Neugebauer (in collaboration with L. Yang and S. Wippermann, GO department): Accurate hydration energies from *ab-initio* calculations

Growth Modelling

L. Lymperakis and J. Neugebauer (in collaboration with Infineon Technologies Austria AG): Identification and strategies to passivate efficiency limiting defects in GaN-based power electronics through *ab initio* simulations

L. Lymperakis, Ch. Freysoldt, S. Maisel, and J. Neugebauer, (in collaboration with M. Albrecht, IKZ, Berlin): *Ab-initio* based cluster expansion simulations of InGaN alloys

L. Lymperakis and J. Neugebauer (in collaboration with Ph. Ebert, Forschungszentrum Jülich): Electronic properties and energetics of novel nanostructures

L. Lymperakis and J. Neugebauer (in collaboration with M. Himmerlich and S. Krischok, TU Ilmenau): Electronic properties and thermodynamics of semiconductor surfaces

L. Lymperakis (in collaboration with A. Georgakilas, University of Crete, Greece): Growth of III-Nitride nanostructures

L. Lymperakis (in collaboration with E. Iliopoulos, University of Crete, Greece): InGaN alloys for photovoltaic applications

M. Alam, L. Lymperakis, and J. Neugebauer (in collaboration with MA and SN): Electronic properties and thermodynamics of point defects in oxide- and organometallic- perovskites

Department of Interface Chemistry and Surface Engineering

M. Rohwerder, M. Stratmann (provisional head J. Neugebauer)

Introduction

The Department of Interface Chemistry and Surface Engineering (GO) is mainly focussing **on corrosion and adhesion science as well as electrochemical energy conversion**. It is internationally known to be one of the leading groups in the field of electrochemical sciences. Our mission is to combine both fundamental and applied sciences to tackle key-questions for a progress towards new or better, energy saving and efficient, cheaper and longer lasting materials for applications in structural (in particular steels and other alloys) and functional materials, e.g. for fuel cell catalysts, batteries, adhesives and smart coatings amongst others. The department currently hosts five research groups. The different groups focus on high-throughput methods and the development of combinatorial methods in adhesion science and electrochemistry, on characterization of electrified interfaces by complementary methods such as vibrational spectroscopy, *in-situ* diffraction studies and scanning probe techniques, such as Scanning Flow Cell (SFC), Scanning Kelvin Probe (SKP), Atomic Force Microscopy (AFM) or Scanning Tunnelling Microscopy (STM), as well as on related *ab initio* simulation. We combine electrochemistry with a surface and interface science approach, and in most projects we complement both, experimental studies on atomically well-defined model systems as well as on technical systems with atomistic *ab initio* modelling. All groups in the department have their independent and strong research agenda, while collaborative research projects are synergistic and focus on major challenges and complex scientific questions that require the scale and interdisciplinarity (detailed below).

In the reporting period the department was subject to a number of advancements and adjustments: First of all, in June 2014 the head of the department, Martin Stratmann, took over as president of the Max Planck Society and is officially on leave from his position at the MPIE. Michael Rohwerder took over the coordination of the department and Jörg Neugebauer (head of the department "Computational Materials Design") acts as temporary head of the department. In 2013 the department was able to gain Stefan Wippermann as head of a new research group on "Atomistic Modelling" (see p. 29). The motivation of this theory group located inside an experimental department is to gain atomic level insight into key processes in the gas-phase, in solutions, at interfaces/surfaces and in nanostructures, which are inaccessible by other means. Moreover, in 2013 Frank Renner (head of the former "Interface Structures and High Temperature Reactions" group) accepted a position as professor at the University of Hasselt and left the MPIE. In 2014 Michael Rohwerder was offered the position as full professor in the MSE department at the Ohio State University, but could be successfully kept at the Institute. The name of his research group was changed from "Molecular Structures and Surface Modification" to "Corrosion" to better cover the much broader current scope of this group. Furthermore, at the end

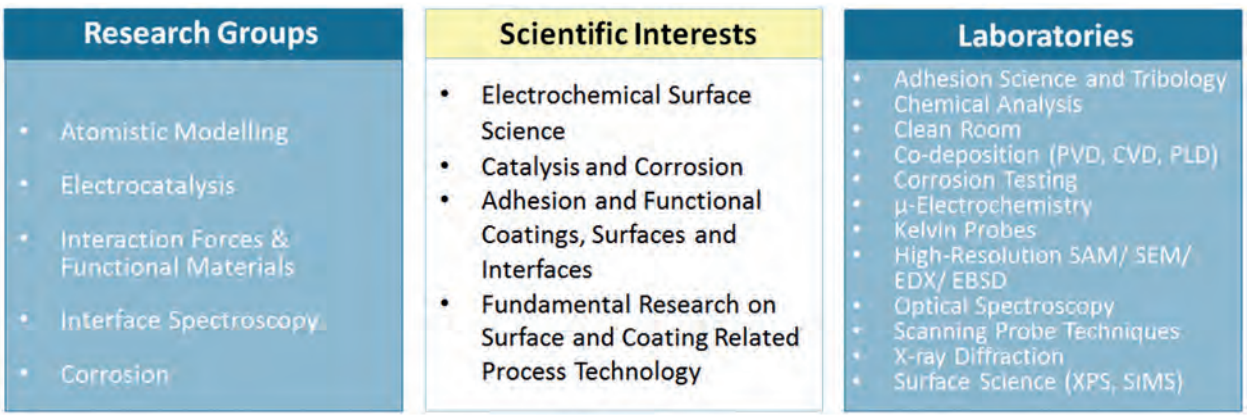

Fig. 1: *Research portfolio and expertise.*

Fig. 2: *The GO (summer 2013).*

of 2014 the Christian-Doppler-Laboratory (CDL) for Diffusion and Segregation during Production of High Strength Steel Sheet (group head: Michael Rohwerder), which was established in 2008, was concluded after seven successful years.

The department is actively participating in various collaborative research efforts with internal and external partners. Several scientists of the department are taking part in the DFG Cluster of Excellence „Ruhr Explores Solvation" (RESOLV), which is centred at Ruhr University Bochum's (RUB) Faculty of Chemistry and Biochemistry. Our contributions to solvation science in RESOLV focus on the role of solvents in electrochemical reactions, and solvation of interfaces. Further, the GO is part of the EU 7th framework programme Marie Curie Initial Training Network (ITN) project „Somatai - Soft Matter at Aqueous Interfaces, which started in October 2013.

With its versatile experimental and theoretical expertise (Fig. 1) the GO is in the unique position to assist and promote diverse **industrial research by its profound expertise in investigating the underlying fundamental electrochemical reaction mechanisms and kinetics**. For instance, electrochemical oxygen reduction reaction (ORR) - a key process in corrosion as well as energy conversion - has been the focus of several joint research projects in the department aiming at a fundamental understanding of its mechanism for better control in corrosion protection as well as improved catalysis in fuel cells and air batteries. These research projects combine both advanced electrochemical as well as *in situ* and in operando spectroscopic experiments with theoretical modelling. In the reporting period besides ORR also the oxygen evolution reaction (OER) has become object of intense research activities and in this context also research on transpassivity of electrode materials under OER conditions. The knowledge obtained in the fundamental research on electrochemical key reactions such as oxygen reduction and oxygen evolution plays a crucial role in helping us to unravel practical problems met in industrial applications or processes such as in corrosion, batteries and fuel cells.

Several research projects focus on industrial processes such as electrophoretic coating, phosphating, alternative surface treatments. Further, considerable research effort is centred on diffusion and segregation during production of high strength steel sheets, including e.g. the complementary experimental and theoretical investigations of grain-boundary oxidation processes. A special collaborative interest of the institute is hydrogen in steel. The activities in this field have been further enhanced, complementing experimental and theoretical methods in cooperation between the departments play an important role. In the GO in particular the Scanning Kelvin Probe and Scanning Kelvin Probe Force Microscopy were further developed in combination with complementing techniques to uniquely and directly detect hydrogen in steel with high spatial resolution (see p. 39).

Scientific Concepts and Broader Impact

All our research groups are synergistically working on common areas of interest and we are strongly dedicated to collaborative work with external partners. Our scientific concept comprises diverse fundamental and industrial fields:

Electrochemical sciences

In the recent years extensive collaborative experimental and theoretical work focussed on the **electrochemical oxygen reduction reaction (ORR)**, a fundamental electrochemical reaction relevant in both corrosion as well as energy conversion processes. At metal surfaces the ORR is the cathodic partial reaction driving many corrosion processes. On the other hand, the electrocatalysis of the ORR in fuel cells and air batteries is intensely studied with the aim of improving the kinetics and reducing the over-potential that limits the energy efficiency. One important approach for advancing our understanding of this reaction is to make progress in *ab initio* simulations about it. This is, however, difficult, because reliable experimental *in situ* data for instance of reaction products are difficult to obtain and thus experimental feedback is more or less missing. To overcome this problem dedicated model experiments were designed. By combining electrochemical experiments with attenuated total reflection infrared absorption spectroscopy, the mechanism of the electrochemical oxygen reduction reaction on n-Ge(100) as a model semiconductor has been investigated. Surface-bound superoxide and peroxide have been found as intermediates both in acidic and alkaline electrolytes. Peroxide is more prominent in alkaline solutions. For the assignment of the vibrational spectra, **a combination of density functional theory (DFT) calculations and isotope exchange experiments was used** [1-2]. Especially in acidic solution, the onset of the oxygen reduction is closely linked to a change in surface termination to an H-terminated surface at negative electrode potentials. On the basis of several experimental datasets, **a catalytic cycle for the ORR on Ge(100) was suggested** [1]. Analysing the relation between absorbance of certain intermediates and total current opens the way for a detailed understanding of the kinetics of individual steps in this multistep reaction [2-4].

In collaboration with the group of P. Koelsch (Karlsruhe Institute of Technology / University of Washington, Seattle), who is an expert on sum frequency generation (SFG) spectroscopy, *in situ* electrochemical SFG experiments on electrode surfaces modified by molecularly highly ordered araliphatic self-assembled monolayers have shown third-order nonlinear optical effects, i.e. a coupling of the static electric field to the vibrational transitions [5]. **Such a coupling may be exploited to probe the electric field at the electrode/electrolyte interface**, if there is a method (e.g. by first principles calculations) to quantify the coupling coefficient. The molecular structure of this electrode/electrolyte interface is essential in electrochemical and natural processes. In particular, ion and water structuring at charged solid/electrolyte interfaces dominate structure and functionality in many physiological, geological, and technological systems. In technological applications and processes ion concentration ranges often above 50-100 mM where structuring is expected to occur within the range of molecular dimensions. Y**et no qualitative or quantitative model exists for predicting ion structuring at solid/liquid interfaces**. In the recent years, we started to use force probe experiments as workhorse to directly probe structural forces at solid/liquid interfaces. For instance we showed how specific ion adsorption can strongly influence how electric charge is compensated in the electric double layer on model ceramic surfaces [6]. These studies are planned to be complemented by experiments with the recently installed Near-Atmospheric-Pressure Photoelectron Spectroscopy (NAP-XPS). The **NAP-XPS** is a new instrument in the department and has now been integrated into a dedicated environment for fundamental research on electrochemical sciences, partly in cooperation with the excellence cluster RESOLV.

Also interfacial structuring of organic electrolytes, including r**oom temperature ionic liquids (RTILs) and Li-ion battery fluids**, was studied. RTILs have emerged as unique electrolytes for energy applications offering potential for designable chemical and physical properties. How ionic liquids structure at charged interfaces determines the functionality in electrochemical devices such as batteries or super capacitors.

Yet, the importance of impurities (water or other solutes) on molecular ion structuring and charging mechanism of solid interfaces in RTILs is unclear and has been largely ignored. Impurities may alter structures, charging characteristics, and hence performance at electrified solid in both a positive or negative way. In the reporting period **force probe experiments and XPS measurements** were utilized to directly measure how water and other impurities alter the interfacial structuring and charging characteristics of RTILs on dielectric surfaces and electrified metal surfaces [7]. On ceramic interfaces water can dissolve surface-bound cations, which leads to high surface charging and strong RTIL layering. In contrast, layering of dry RTIL at weakly charged mica surfaces is weakly structured. At electrified gold electrodes the influence of water is limited to interactions within the RTIL layers, and is not related to a direct

electro-sorption of water on the polarized electrode. Currently, the influence of other potentially beneficial additives such as organic long-chained molecules and polymer materials is tested. Generating such detailed insights into molecular interface structures will further guide the targeted development of structures and properties at electrified interfaces.

Another important aspect is **how electric double layers respond dynamically during active operation** of an electrochemical device, or during ongoing active corrosive processes that continuously generate or deplete charge at an interface. To study such dynamic aspects of electric double layers we also utilized direct electric double layer force measurements. For the first time we could directly measure strong electrochemical reaction forces, which are due to temporary charge imbalance in the electric double layers caused by depletion/generation of charged species. The real-time capability of our approach revealed significant time lags between electron transfer, oxide reduction/oxidation, and solution side reaction during a progressing electrode process. Comparing the kinetics of solution and metal side responses provided unique evidence that noble metal oxide reduction proceeds via a hydrogen adsorption and subsequent dissolution/re-deposition mechanism [8]. In addition, the existence of reactive forces may explain why adhesive and cohesive forces can trigger processes such as crevice corrosion or stress corrosion cracking and nano-particle from electrode support materials.

Many of the research projects allocated in the field of electrochemical sciences are closely related to the DFG-funded Cluster of Excellence RESOLV. More specific current research within RESOLV is, among other activities, focussed on electrochemistry in the “dry” (see further below) and on *in situ* vibrational spectroscopy, with the aim on the understanding of the electrode-potential dependent solvation of electrodes [9]. Main aim is again to link experimental results to first principles calculations.

Corrosion

The corrosion research of the department includes aqueous, atmospheric and bio-corrosion processes and their inhibition, covering both fundamental and applied aspects.

Using the scanning flow cell (SFC) system with downstream analytics allows **electrochemical high-throughput screening and characterization of corrosion properties of material samples**. This method, which was developed in the GO, has become a routine technique for corrosion research and up to now 8 set-ups with integrated mass spectroscopy or UV-vis analysis are in operation. In the reporting period SFC was successfully applied for studying the corrosion of magnesium, where it provided important insights, including the much disputed negative difference effect [10-11]. In extension, current efforts include the investigation of various material libraries, which should finally lead to guidelines for the optimization of material composition for best corrosion protection with regard to the respective environment of use.

Of special importance of our research is the corrosion behaviour of zinc (alloy) coatings. Despite the high importance in corrosion protection, the fundamental understanding of the behaviour of zinc based metallic coatings under different and often changing environmental conditions is still not exhaustive. Therefore, the in-house developed SFC high throughput approach coupled to online analytics, which is capable to deal with the issue of the complex interrelation between many material parameters and simulated test conditions efficiently, has been in particular extended for the variation of electrolyte composition. This has been utilized in collaboration with industrial partners to increase our understanding of the impact of the electrolyte components on the fundamental corrosion mechanism and kinetics of Zn based systems [12]. Moreover, the SFC has been successfully installed in the laboratories of the collaboration partners, and is being further technically optimized so that it can become a routine tool for the evaluation of corrosion properties also in other industrial laboratories.

The investigations by SFC are mainly focused on the fundamental dissolution kinetics. The **longterm corrosion performance** of zinc alloy coatings is, however, to great extent also determined by the corrosion product layers forming over time. These were in focus of research, too. Important information on the effect of environmental factors and the role of the micro-structure could be elaborated [13-16]. Moreover, also the **initial stages** of Zn corrosion are of importance, as they may influence the further course of corrosion. Electrochemically grown oxides on zinc are the first corrosion products. A combination of ex situ and *in situ* analysis of the oxidation of zinc in carbonate shows that the oxide films growing are significantly different from bulk oxides, as e.g. detected via their Raman and photoluminescence spectrum. The reason is the large density of defects in these oxides [17]. On copper, oxide growth in solution has implications for the antibacterial activity of the copper surfaces, as studied in collaboration with F. Mücklich, Chair of Functional Materials of the Saarland University [18]; however, these are non-trivial effects that require further model experiments.

The corrosion of metallic alloys, especially steels, in the presence of aqueous H_2S, so-called **“sour gas corrosion”**, is an old topic in corrosion research that surfaces again because of the exploitation of more

and more non-classical sources of oil and gas. When reviewing the literature, one notices a lot of reports based on field experience and standardised tests, but there is still a limited understanding of a number of fundamental aspects [19]. The limited understanding motivated collaboration with the steel industry to investigate in more detail mechanistic aspects of sour gas corrosion, e.g. the electrochemistry of iron in acidic electrolytes containing H2S. Interesting results show the metallic nature of the corrosion products, and a strong oxygen content in corrosion products, possibly caused by the presence of amorphous iron oxides [20]. The complex chemistry of iron sulfides and oxides, coupled with a complex electrochemistry makes sour gas corrosion hard to understand, and current efforts are directed to further progress in this direction.

Microbially influenced corrosion (MIC) by marine sulfate-reducing bacteria is a major contributor to corrosion of iron in anoxic environments [21]. Anaerobic MIC causes serious damages in the oil and gas industry, thus assessing and monitoring of corrosion problems and also elucidating the yet still unresolved corrosion mechanism is of great importance. In close cooperation with the Max Planck Institute for Marine Microbiology in Bremen and in a multidisciplinary approach utilizing electrochemical techniques, surface analytics and molecular biological methods, we succeeded in quantifying corrosion rates *in-situ* [22] and gaining a more detailed insight into the fundamental electron transfer mechanism at the electrode/bacteria interface [23-24]. More recently, we have also shown that the direct electron transfer mechanism also proceeds in other bacterial cultures, in particular methanogenic lithoautotrophic archaeon, which makes them highly active and selective in the conversion of CO_2 to CH_4, a topic also of great importance in energy conversion [25].

Crevice corrosion (CC) of metals remains a serious concern for structural materials and aerospace engineering. Yet a **real-time** *in situ* **visualization of corrosion, and its inhibition within a confined geometry**, remains challenging. In our department we recently demonstrated how white light interferometry (WLI) can be utilized to directly visualize corrosion processes in real-time, *in-situ* in a confined (i.e. buried) geometry [26]. We studied in detail how pure **aluminum corrodes in crevice geometries and how vanadate ions can effectively inhibit CC of aluminum**. As shown in Fig. 3 (a) corrosive 5 mM NaCl solution is sandwiched between the aluminum oxide and an opposing crevice former surface (mica) to form a confined zone. Simultaneously WLI directly reveals the shape of a confined crevice area in terms of fringes of equal chromatic order (FECO) – shown in the panels above the schematic. A FECO is a standing wave that reflects back and forth between the corroding aluminum surface and the inert probe mirror located behind the crevice former (mica). After 1.5 and 2 hours, Fig. 3 (b-c), clearly show that regions just outside the intimate contact area show first signs of corrosion (increased light intensity). Interestingly, CC does not initiate at the intimate contact zone but just outside, where the electrolyte layer above the Al is about 20-200 nm thick. This behaviour indicates a delicate balance between the established corrosive potential within the confined zone and material transport rates out of/ into the confined zone. Fig. 3

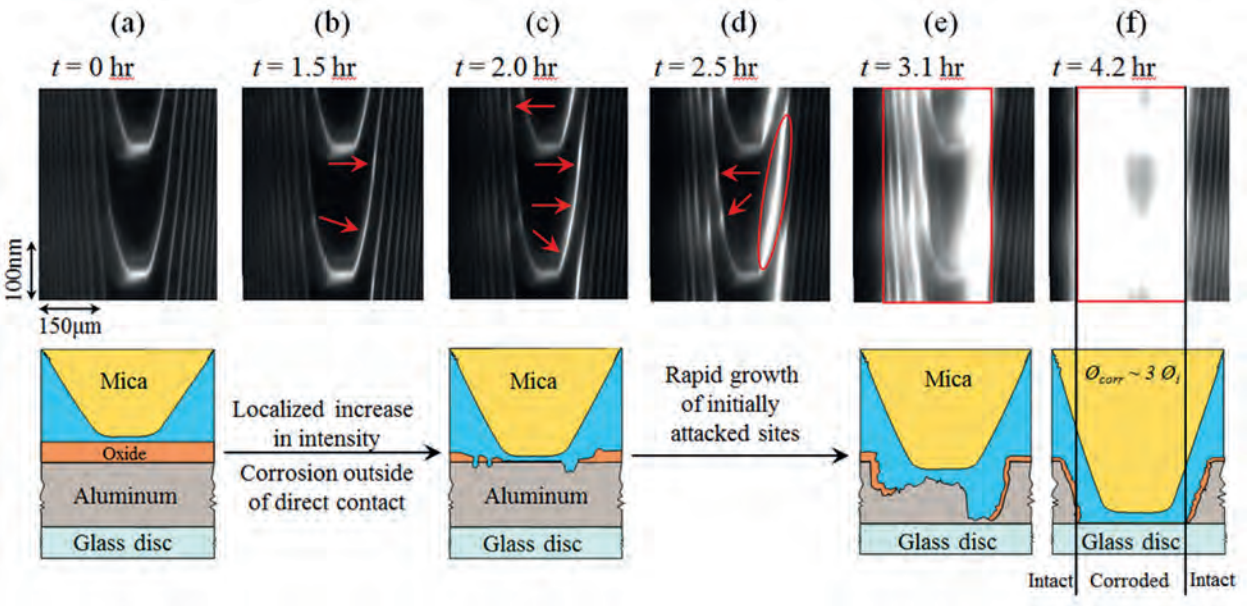

Fig. 3: *Consecutive 2D FECO images obtained as a function of time after injection of 5 mM NaCl into a confined aluminum/mica contact. The schematics below show progress of the corrosive reaction as deduced from the FECO images. As indicated in the schematic shown in (c) a subtle balance between material transport rates (diffusion and migration) as well as reaction rates may control the locations where rapid Crevice Corrosion initiation is most likely [26].*

(d-e) show how the confined zone rapidly corrodes until the corroded area is about three-times the initial intimate contact area. Using this method we could directly quantify (1) critical bulk concentrations of the corroding species (chloride) that are necessary to initiate CC; (2) the concentration of corrosion inhibitor above or below which the corrosion is effectively inhibited For instance, 2.5 mM NaVO3 can effectively inhibit the corrosion of aluminum in 5mM NaCl solutions for 25 hours, however, in 50 mM NaCl the rapid breakdown of the native oxides occurred after about three hours. (3) In general we could show that CC initiates with a breakdown of the passivating oxide surface. This method now allows for a detailed and high throughput screening of effective corrosion inhibitors.

Such a real-time Angstrom-resolved **visualization of dynamic processes at electrified solid/liquid interfaces** has not been feasible to date. We recently also reported a unique experimental setup that allows us to generate a real-time atomistic view into dynamic processes at electrochemically active metal interfaces using white light interferometry (WLI). Quantitative *in situ* analysis of the potentiodynamic electrochemical oxidation/reduction of noble metal surfaces shows that Angstrom thick oxides formed on Au and Pt are high-ik materials; that means, they are metallic or highly defect-rich semiconductors, while Pd forms a low-ik oxide. In contrast, under potentiostatic growth conditions, all noble metal oxides exhibit a low-ik behaviour [8]. This clearly demonstrated that surfaces under active conditions are very much different from equilibrated surfaces. Yet, exactly the dynamic aspects of growing or reducing oxide thin films are very important with respect to stability of metallic materials. With our new methods we can now for the first time aim to understand the molecular origin of actively progressing processes such as reactive dissolution of metals, in particular also in trans-passive regions, where passivation typically breaks down during dynamic change of the surface structure.

With respect to trans-passive degradation, the department combines a number of different techniques in order to study how and why oxides break down. This is becoming a topic of increasing importance for all research groups of the department who strongly cooperate on this topic.

High temperature oxidation is another topic that is becoming increasingly important within the GO. Special focus are short term high temperature treatments that are crucial in many industrial processing steps in steel making, such as hot rolling and recrystallization annealing before hot dip galvanizing. These relatively short processing steps are generally not much investigated yet and are determined by kinetics of oxygen uptake, nucleation and growth of oxides [27] and only to limited extent by diffusion, usually considered of key importance in high temperature oxidation, which leads to final morphologies that are still far from equilibrium. This research was originally part of the Christian Doppler Laboratory for Diffusion and Segregation during the Production of High Strength Steel Sheet (Michael Rohwerder) and will be continued in the Corrosion group.

Adhesion, thin films and friction

Organic coatings are commonly employed to protect materials surfaces against corrosion. On steel, including galvanised steel, cathodic delamination is the main mechanism of failure of these coatings. As chromating is already widely banned and now also **phosphating** is foreseen to be applied to much lesser extent in the near future, the interface between organic or hybride organic-inorganic coatings and the metal surface become more and more important. **Delamination at such interfaces is one of the key expertizes of the department.**

Recent efforts have been made to understand the nature of the chemical reactions that occur in the process of cathodic delamination by preparation of synthetic model interfaces, mainly on zinc, that have been polymer coated and subjected to cathodic delamination. After deposition of ZnO sol gel films with different morphology on zinc surfaces, those morphologies with mainly low energy surfaces show slowest delamination of weakly bound polymer coatings, indicating that the destruction of the ZnO surface is important [28]. On the other hand, thin acrylate polymer films have been prepared in a free radical copolymerisation process where one co-monomer is bound to the zinc surface. Resulting reaction-controlled delamination rates depend e.g. on the content of hydrophobic cross linkers and the total crosslinker content, which implies that a role of radical intermediates of the ORR is likely in the delamination process [29]. *In situ* Raman monitoring of the initial stages of cathodic delamination on zinc under certain conditions shows oscillations in pH and amount of corrosion products. The observation of oscillations implies that anodes and cathodes must be correlated over the surface, as opposed to the current textbook picture of random locations [30].

The breaking of the covalent bond between gold and the sulphur atom of a self-assembled monolayer (SAM) may be regarded as one particular mechanism of de-adhesion. In general self-assembled monolayers can serve as model systems for studying degradation mechanisms as they might occur at buried interfaces. Hence, a number of self-assembled monolayers that could be of interest for further studies was investigated [31-32]. In a series of experiments of the reductive desorption of SAMs in a coupled el-

lipsometric – electrochemical experiment, araliphatic and alkyl SAMs with long chains have been found to remain intact or even adsorbed to the metal surface even after breakage of the covalent bond [33]. On the other hand, shorter thiols stabilise aggregates possibly containing hydrogen at the electrode/electrolyte interface [34]. Up to now one unsolved hindrance for a detailed study of fundamental investigation of cathodic delamination was that the oxygen reduction rate at the buried interface was not directly accessible. Based on combining Kelvin probe with a hydrogen permeation experiment, a novel methodology was developed which allows for the first time direct measurement of the oxygen reduction kinetics at the buried interface (see p. 38). Also of interest and of crucial importance for understanding delamination is the role of surface oxide terminations and studying its effect on the properties of the resulting interface with polymers [102]. Another important aspect of delamination is the mobility of charges along the buried interface. Hence, the study of charge mobility and of its dependence on crucial surface parameters such as OH termination is of great importance [103, 109].

In addition, unravelling the complexity of modern adhesives acting in the macroscopic world relies on understanding **the scaling of single molecular interactions towards integral macroscopic interactions**. In our department we recently developed a synergistic experimental approach which combines macroscopic adhesion measurements using a Surface-Forces-Apparatus and single molecule unbinding experiments using an Atomic-Force-Microscope (AFM) [35]. We developed a unique experimental framework to test the well-renowned Jarzynski's equality, which relates work performed under non-equilibrium conditions (in this case during single molecule unbinding in AFM) with equilibrium free energies, which are necessary to predict macroscopic interactions. In two case studies it has been shown that the equilibrated macroscopic work of adhesion scales linearly with the number density of interface bonds s as long as the chemical functionalities do not interact with each other laterally. Irrespective of how far from equilibrium single molecule experiments are performed, the Jarzynski's free energies converge to the same values as measured on a macroscopic scale. These results validate the applicability of Jarzynski's equality in general, and allow us now to unravel the scaling of non-equilibrium single molecule experiments to scenarios where a large number of bonds interacts simultaneously in equilibrium and at the macroscopic scale. Based on this we developed a scaling strategy that allows us to predict large-scale properties such as adhesion at electrified interfaces on the basis of single-molecule measurements (Interaction Forces and Functional Materials group) [36]. This now opens a new path to understand macroscopic adhesion and delamination.

Functional surfaces, interfaces and coatings

The development of **intelligent coatings for corrosion protection** within the department focuses to a significant extent on the application of conducting polymers and particle modified zinc coatings. While in the prior reporting period a thorough investigation of the problems involved with the use of conducting polymers for corrosion protection has been carried out in depth and solutions how to solve them were developed, in this reporting period further developments were made for a more efficient performance of so called intelligent self-healing coatings. One main success was the development of polyaniline capsules that can be loaded with inhibitors or other self-healing agents (together with partners from the Max Planck Institute for Polymer Research in Mainz) and first successful applications [37-38]. Another major break-through was the successful combination of a smart organic coating containing smart capsules loaded with monomer with a zinc coating containing capsules that were loaded with a catalyst [39]. For the first time a coating system could be demonstrated to case-sensitively release active agents upon onset of corrosion that closed a macroscopic defect site by formation of a new polymer coating.

Moreover, thin organic films have been exploited for surface **modification of metal surfaces**, combining innovative chemical synthesis in collaborating groups with high-level surface analysis at the MPIE. Salt-like Fe^{II} containing complexes were immobilised on gold via thiocyanate anchors in a collaborative work with A. Grohmann, Chair of Bioinorganic Chemistry, TU Berlin [40]. Phenothiazines as redoxactive components and as candidate materials for molecular electronics have been synthesised with phosphonate linkers in the Department of Organic Chemistry at the Heinrich Heine University Düsseldorf, headed by T.J.J. Müller. Such phenothiazines adsorb as monolayers to oxide-covered iron and as multilayers to oxide-covered zinc [41], which widens their spectrum of applications. Also, the classical gold-sulphur system still holds surprises when used with complex molecules, e.g. azobenzene derivatives. Ordered films with different adsorption geometries have been obtained here, depending on the precursor, but with same chemical composition [42].

Besides their role in corrosion and corrosion protection, particular in passivity, semiconducting oxides are also interesting for a number of other applications, e.g. in **photovoltaics, photocatalysis and in sensing**. For a fundamental understanding of the role and nature of defects as well as the band alignment, advanced photoemission spectroscopy experiments in ultrahigh vacuum have been conducted in collaboration with M. Krzywiecki from the Silesian University of Technology, Gliwice, Poland. As a result, detailed band diagrams have been experimentally determined

for sol gel films of ZnO [43] and SnO_2 [30]. Results indicate that such films are extremely oxygen deficient. For ZnO, defects must be present which serve as acceptor, donor and trap at the same time [43]. A new method for the detailed analysis of the angle dependence of X-ray photoelectron spectra has been developed for the ex situ characterisation of the electronic structure of thin semiconducting films [30].

The presence of defects in a wide bandgap semiconductor manifests itself in the photoluminescence (PL) spectra. For ZnO (band gap ~3.4 eV), PL is now observed also after excitation below the bandgap, e.g. in the visible. In spherical ZnO micro-resonators, this PL can couple to whispering gallery modes. The shift of such modes in turn can be used to sense the refractive index of the surrounding medium [44]. Absorption of visible light of ZnO micro- and nanostructures is also facilitating photocatalytic reactions, as shown for the decomposition of an organic dye. Interestingly, the ZnO photocatalysts produced for this study have been prepared by cathodic delamination, i.e. a corrosion process [45].

Metal colloids are frequently used as electrocatalysts. A new synthesis strategy for gold particles without organic capping agents from a mixture of water and dimethylformamide has been systematically exploited. By variation of the solvent composition, particles with different morphologies were obtained. At low water content, particles with the catalytically active Au(110) dominate [46].

Measurement and targeted **steering of molecular interaction forces is another fundamental necessity to understanding stability and synthesis of novel functional interfaces and coatings**. In particular, interactions between hydrophobic groups are fundamental in self-assembly and hierarchical structuring of soft matter. The molecular origin of hydrophobic interaction forces is however still not fully revealed, and seems to strongly depend on how water dipoles are arranged around hydrophobes. We recently confirmed experimentally that the hydrophobic force law, which characterizes the interaction of two hydrophobes in aqueous electrolytes, is both long-ranged and exponential down to distances of about 1–2 nm over large concentration regimes from 1 mM to 1 M salt concentrations [47-48]. In addition, we utilized functional carborane self-assembled monolayers to directly tune the molecular dipole moments of water molecules at hydrophobic interfaces. Our data showed that dipoles that are oriented parallel to a hydrophobic surface-plane can induce very long-range interaction forces due to lateral formation of giant dipoles [49]. Hence, surface dipoles may additionally lead to an orientation of water molecules at hydrophobic surfaces.

Another important aspect of functional materials are the swelling/shrinkage dynamics during exposure to different environments. This includes for instance release of molecules from porous media as well as the swelling of organic coatings. For model studies of such swelling dynamics we used Metal-Organic Frameworks (MOFs) which are three dimensional (3D) crystalline coordination polymers consisting of metal ions linked by organic ligands. Gas adsorption in MOFs crystals can dramatically affect their size (expansion and/or shrinkage) or lead to distortion of their porous structure/framework. This behaviour can strongly affect the performance of MOF-based gas storage devices. We showed how white light multiple beam interferometry (MBI) allows to measure in real-time (msec time resolution) the deformations (Å distance resolution) of MOF crystals during cyclic changes between an inert gas (Ar) and humidity. Dynamic and non-monotonic deformation behaviour (contraction/expansion) due to gradual filling of the different adsorption sites present in the unit cell of the crystal was measured for the first time *in-situ* with high time resolution [50]. These studies will now be extended into the measuring of hydrogen loading/ unloading kinetics of various MOF systems as well as to study shrinkage/expansion of e.g. organic coating on corroding metal surfaces.

Industrial processes

In collaboration with different industrial partners, the GO continued to work on fundamentals of the formation of **conversion coatings**. Phosphating is still the most frequently applied pre-treatment process, but requires special attention on new metallic coatings and on modern steels. Electrochemically assisted phosphating is one option to obtain homogeneous phosphate coatings on inhomogeneous substrates, and also on high-strength steels [51-52]. Detailed investigations of aluminum silicon coated steel contribute to the puzzle for understanding the exact role of the titanium phosphate activation bath. Scanning Auger microscopy shows a phosphate distribution after activation that is reverse to the distribution of zinc phosphate crystals after phosphating [53]. Statistical analysis of the size of phosphate crystals after different times of electrochemically triggered phosphating shows that the activation leads to a slower and more homogeneous growth of phosphate during phosphating. Crystals on non-activated surfaces appear to become larger after shorter phosphating times. Overall, there is a strong effect of the activation bath on phosphate growth, but nucleation appears to be less affected [51].

Nanoceramic, e.g. ZrO_2-based conversion coatings are bound to replace phosphating in the future. In collaboration with partners of the chemical industry, the role of Cu^{2+} added to the deposition solution on the formed conversion coatings was investigated. It turns out that the corrosion-promoting Cu^{2+} enhances

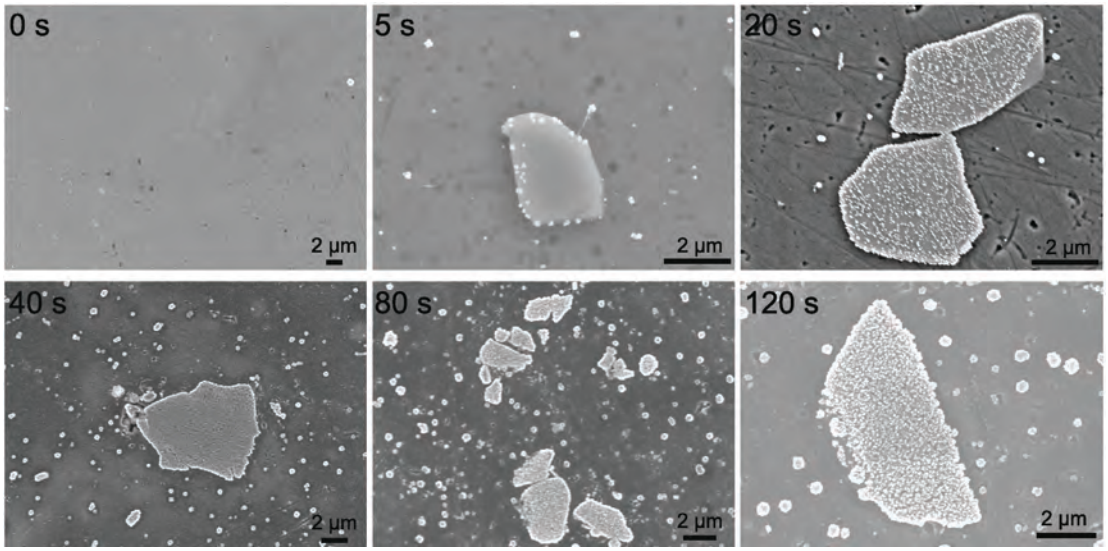

Fig. 4: *SEM images of pretreated AA6014 substrates after different immersion time [54].*

deposition of the conversion coating around intermetallic particles, and at grain boundaries (Fig. 4). This "controlled corrosion process" during conversion coating formation may be crucial in the protection of the inhomogeneous surfaces in "real" materials [54]. Further recent activities include an investigation of the changes in the oxidic conversion layer after electrochemical polarisation.

Joining different materials by welding is an important industrial process, but some material combinations are not accessible in the classic welding processes that involve melting. In collaboration with the Institute of Production Engineering and Forming Machines of TU Darmstadt headed by P. Groche within the DFG-funded priority programme SPP1640 "Joining by forming", the role of the interface chemistry on cold welding of steels and aluminum alloys is being investigated. Primary heat treatment of the partners critically influences the mechanical properties of the surfaces, and hence affects the bond formation [55]. On the microscopic and nanoscopic level, a thin reaction layer consisting of Fe and Al was found at the interface between steel and aluminum alloy [56], that may be critical for the adhesion, i.e. weld formation. The exact nature of this layer is subject of current investigations. Likewise, the corrosion behaviour of such cold-welded structures is currently being investigated. Attempts to create a simple model experiment that permits studies of well-defined samples to extract essential physicochemical parameters in the cold welding process are a further field of work [57].

Moreover, zinc based metallic coatings are of tremendous importance for corrosion protection and are object of research since decades. Predicting the long term performance of novel zinc alloy coatings is still a problem (see Corrosion above). A new challenge is the so called hot stamping. The development of metal coatings that are suitable for that process and still provide reliable cathodic protection and good long term corrosion performance is the main target of a project financed by the Federal Ministry of Education and Research (KOWUB). The main activity of the MPIE is to investigate the potential of iron rich Fe-Zn-Mg alloys.

The fully automated SFC has been also extended for the analysis of real, high surface-area electrocatalysts, which are important in electrochemical energy conversion devices such as fuel cells and electrolysers. This has been highly beneficial as the wide parameter-space for material composition and structure as well as operation conditions require also fast screening techniques to obtain reliable information within a reasonable timeframe. The SFC has been shown to reliably acquire the activity and the stability of noble metal catalysts with high-throughput [58], and is currently employed for a wide range of different types of porous materials including exciting non-noble catalysts for oxygen reduction [59].

Fundamental problems of oxidation and hydrogen uptake during industrial production steps of high strength steel sheet have been the focus of the Christian Doppler Laboratory of Michael Rohwerder.

Scientific Groups

Electrocatalysis (K. J. J. Mayrhofer)

The research interests of the Electrocatalysis group (www.mpie.de/ecat) are related to electrochemical reactions at the solid-liquid interface, both for corrosion processes and electrochemical energy conversion. The main focus of the group is placed on the concerted investigation of the activity, stability and selectivity of electrode materials for such heterogeneous electron-transfer reactions. Thereby the behaviour of well-defined and real material surfaces are investigated and compared in order to achieve a fundamental understanding of the decisive processes and structural effects. This is achieved by a unique combination of electrochemistry with complementary techniques for surface characterization and reaction product determination.

The new electrochemical methods, which have been developed in the group over the last years [58, 60-61], are utilized to investigate a wide range of scientific challenges. High-throughput combinatorial screening tools combined with sophisticated automation and advanced methods for data evaluation and processing are central for the more systematic and reliable investigation of a large number of samples. In addition, coupling electrochemistry with online reaction product determination by Inductively Coupled Plasma Mass Spectrometry [61] and Differential Electrochemical Mass Spectrometry [62] increases the information depth significantly.

These advanced techniques have provided new exciting insights into processes at the solid-liquid interface particularly of materials for electrochemical energy conversion. The key reactions studied in our laboratory include the oxygen reduction reaction (ORR) and evolution (OER), as well as the utilization of CO_2 by electrochemical means for the production of so-called solar fuels [63]. In contrast to the plain activity evaluation of catalyst materials that dominate the literature in the field, we focus on the overall performance including stability and selectivity, as operation over extended times is crucial for the success of fuel cells and electrolysers. Namely, the conditions during the reactions in these devices are often quite harsh and lead to corrosion of the catalyst material, even though they typically consist of noble metals. Pt, which is among the most active materials for the ORR, for instance dissolves significantly during transient operation when the surface alternates between reduced and oxidized condition [64-66]. Au instead dissolves continuously and to a major extent during steady-state operation at positive potentials close to the oxygen evolution, since it does not form a passivating oxide layer as Pt [67-70]. All noble metals have in common that they dissolve to a certain extent, but clearly there is no inverse relationship between activity and stability as commonly believed [71]. When noble metals are alloyed with transition metals to enhance the intrinsic activity, the dissolution becomes more complex, yet still the performance can be resolved with our special techniques [72-73]. Indeed, only in these investigations of material libraries the full potential of the approach becomes obvious, which will in future also be further extended to the investigation of different catalyst materials like the promising Ru and Ir oxides for the OER [74-75].

Besides these studies on rather model like electrode surfaces, we are also highly interested in real, high surface area catalysts as typically employed in real reactors. The aim is to additionally enhance the fundamental understanding of the structural effects on performance, in order to derive catalyst design principles and achieve optimal operation in applications [76]. In joint efforts with various expert material science groups we therefore contribute to the development of new catalysts, eventually with lower content of scarce noble metals. For instance, together with the department of F. Schüth from the Max-Planck-Institute für Kohlenforschung the concept of “confined space alloying” has been introduced, providing alloy catalysts with unprecedented structural and chemical stability [77-78]. Furthermore, in collaboration with the National Institute for Chemistry in Slovenia, we have demonstrated the beneficial effect of ordered alloy nanoparticle catalysts [79-80], while with the TU Berlin we could show the formation and general instability of nanoporous alloys [81]. Non-noble metal catalysts like the exciting examples of F. Jaouen from the University Montpellier have been recently majorly improved and therefore received enormous attention, however the stability still remains a crucial issue [59, 82]. Exactly therefore, the parallel study and the enhancement of our understanding on activity, selectivity and stability will remain of high importance in electrocatalysis for energy conversion.

Atomistic Modelling (S. Wippermann)

The group was established in February 2013 and is performing *ab initio* theory in the otherwise experimental GO department. The group works in direct collaboration with experiment to gain insights into key processes at solid-solid and solid-liquid interfaces, nanostructures and in the gas phase, which are inaccessible by other means. Employing predictive *ab initio* modelling techniques based on density functional theory and beyond, the group focuses on the general fields of materials for solar and chemical energy conversion and storage. For further details see p. 29.

Interface Spectroscopy (A. Erbe)

The Interface Spectroscopy Group continues to work in two directions, (1) the design of interfaces for spectroscopic investigations and application of spectroscopic techniques to study materials surfaces *in situ* and operando and (2) chemical modification of materials' interfaces to tailor surface properties and to investigate failure mechanisms. Several results within the main focus of the department have already been highlighted in the departmental report.

In the optical development part of the group's work, a new direction involved the use of whispering gallery modes (WGMs) in spherical microresonators from oxide semiconductors as relevant in corrosion. Via defect-related light absorption, photoluminescence can be excited in the visible which couples to the WGMs. Results are emission spectra with narrow lines, observed in ZnO and TiO_2 [44, 83]. It is hoped that using WGMs, highly sensitive optical detection of processes at semiconductor interfaces may become possible. Another major advance was achieved in collaboration with the group of C.F. Chou, Academia Sinica, Taipei, Taiwan. Nanogap electrodes were integrated with Raman spectroscopy, which enabled the trapping and spectroscopic detection of individual protein molecules [84]. A similar approach coupled to electrochemical reactions may enable the understanding of electrochemical processes on the molecular level. Scattering of light is an extremely important phenomenon when considering "real" materials. Continuing a collaboration with R. Sigel, currently at the German University in Cairo, Egypt, ellipsometric dynamic light scattering was developed to extract dynamic information of incoherently scattered light in the presence of strong coherent scattering [85], exploiting the analysis of polarisation of light.

Light is not only used to spectroscopically analyse surfaces, but can also be used for different purposes. In high temperature corrosion, optical heating is frequently used. However, heating efficiency depends on the light absorption. In a comparison between surfaces of different roughness, a model was established which takes into account the scattering from rough surfaces and enables an analysis of the light absorption, hence heating, of metals [86]. Also photocatalysis critically depends on the availability of light. Using a corrosion process, ZnO nanostructures were prepared, in which the combination of the defect-related absorption of visible light with the morphology leads to an almost black material. Thus prepared structures are photocatalytically active [45].

The group's expertise in vibrational spectroscopy of interface dominated materials led to active collaborations with the groups of M. Muhler and W. Schuhmann at the Ruhr University Bochum. We contributed both to understanding and practical analysis of the Raman spectrum of graphene [87], as well as the characterisation of graphene and other sp^2 carbon compounds in complex multicomponent materials [88-91]. New collaborations were also established with groups at the Heinrich Heine University Düsseldorf, in organic chemistry [41] and experimental condensed matter physics [92].

New insight into the chemistry of cathodic delamination processes came from the synthesis of acrylate model polymer thin films with well-defined linkage to the interface. Results show that the delamination is controlled by reaction kinetics, but depends on cross linking and hydrophilicity of the polymers, which all had a thickness in the range of ~30 nm. On the other hand, a covalent linkage to the metal significantly reduces the delamination rate [29]. Consequently, several processes must contribute to the overall delamination rate. A further interesting new aspect of cathodic delamination is the observation of chemical oscillations in the amount of corrosion products and in pH by *in situ* and operando Raman spectroscopy. This observation can be explained with the small reaction volume between polymer and metal during delamination. Because of the consumption of water in the oxygen reduction, the confined region at the polymer/metal interface becomes strongly alkaline. In turn, this stops oxygen reduction, leading to a cyclic behaviour (Fig. 5) [93].

The group contributed actively to the Marie Curie Initial Training Network Somatai by the organisation of training events, participation in organisation of the summer school, and contribution of two chapters to a special volume of tutorials in the series Lecture Notes in Physics.

Christian Doppler Laboratory for Diffusion and Segregation during Production of High Strength Steel Sheet (Michael Rohwerder; until Dec. 2014)

The main focus of this lab, which was successfully concluded in 2014, was on fundamental diffusion and segregation problems encountered during the different production steps of high strength steel sheet. Cooperation partners were e.g. the TU Wien (where the P (Pickling) module was carried out which dealt with pickling after hot rolling). The technical motivation behind this lab was that the development of high strength steels with their characteristic alloying element composition leads to new challenges for the production and processing of steel sheets in order to meet the product requirements. The focus here was on selective grain boundary oxidation during hot rolling and its consequences for pickling, and on hydrogen detection and its uptake kinetics in different process steps. The related questions are of

significant scientific interest and the related research of considerable experimental challenge. In sum these problems are addressed within the lab modules:

SE (Selective Enrichment) Module:

Within this module the activities focused mainly on two approaches: fundamental investigation of grain boundary oxidation based on dedicated model alloys and developing a new simulation tool for describing grain-boundary oxidation on a theoretical level, which, however, was successful only to a certain degree [94]. The reason for this is that the assumption of only diffusion of oxygen and thermodynamics of the oxidation reactions to be considered for a simulation of internal oxidation was not sufficient. In dedicated model experiments, for which a high performing high temperature lab was built up [[95-96]], it was found that for the relatively short reaction times to be considered here, the uptake kinetics at the surface play an important role and that these are determined to a great extent by some alloying elements [27].

In general certain combinations of some of the key alloying elements in high strength steels were found to be responsible for significantly enhanced internal oxidation. This is partly due to their effect on the oxygen uptake kinetics and partly also to the effect of the least noble alloying elements as pioneering oxide former, providing nucleation sites for further oxide growth. Unusual high oversaturation values of alloying elements remaining unoxidized in the matrix were measured [97].

H-Module:

The hydrogen uptake of the material is a significant problem especially for high strength steels, as small amounts of hydrogen in the range of ppm can cause retarded brittle fracture. Uptake during several wet processing steps as well as corrosion and recrystallization annealing is investigated. For the hydrogen uptake during the latter, it was found that similar to oxygen uptake at high temperatures, also the hydrogen uptake is affected by some alloying elements and by the oxygen activity (i.e. dew point) [27]. Furthermore, the novel method for hydrogen ultra-sensitive hydrogen detection with high spatial resolution based on Kelvin probe developed in the prior reporting period was applied to a number of materials for characterisation of hydrogen distribution and its role on embrittlement, as well as for hydrogen uptake during corrosion [98-100]. For a full characterisation, however, it is necessary to combine different techniques, including the novel thermo-desorption set up for high sensitive analysis of hydrogen trapping [101] and Time of Flight – Secondary Ion Mass Spectroscopy ToF-SIMS, see also method development Hydrogen Mapping.

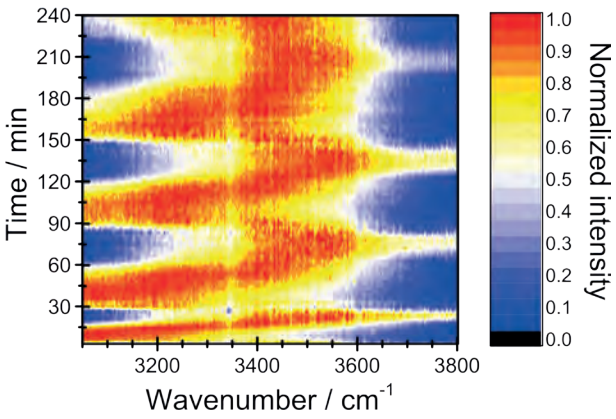

Fig. 5: *Time evolution of false coloured Raman spectra of the OH stretching mode region in the initial phase of cathodic delamination of poly(vinylbutyral) on zinc in the presence of 1M KCl [93].*

Corrosion (Michael Rohwerder)

The main scope of this group is to address fundamental questions of corrosion, surface and coating technology by isolating the crucial problems behind them and designing model experiments and model samples for their systematic investigation. Two major research projects in the group were carried out in the highly competitive framework programme of the Fraunhofer Society (FHG) and Max Planck Society (MPG) collaborative projects. One project ended within the reporting period ("Active Coatings", see below self-healing coatings) and the other one started in 2014 ("Initial Wear", see p. 145).

The further main activities on the research interests in the Corrosion group can be summarized as follows:

1. Elementary steps of electrochemically driven de-adhesion of organic coatings
   Two main approaches are used in the group for studying the fundamental steps of delamination. One is to apply Scanning Kelvin Probe Force Microscopy (SKPFM) for studying microscopic and submicroscopic processes during delamination. The other approach is to investigate the effect of modifications of the surface oxides and/or the functionality of the organic coating on the delamination behaviour. The latter is mainly done by investigating the effect of well characterised self-assembled monolayers [31-33]. However, for an in-depth fundamental investigation of the processes underlying delamination, information about the interfacial reaction kinetics is indispensable, which so far has not been accessible. Currently, a novel method is being developed, which combines hydrogen permeation and Kelvin probe (see p. 38). First results on model samples, including self-assembled monolayer films at the interface, show that this novel method is indeed

able to provide direct information on the oxygen reduction rate at the buried interface.Further, the effect of different pre-treatments on the interface with different coatings and their effect on ion mobility was studied in detail for aluminum [102-103].

2. Electrochemistry in the “dry”
The novel method for hydrogen detection by Kelvin probe relies on ultra-thin palladium films that are evaporated on the surface of the material to be investigated [98]. Over time the hydrogen entering from the sample underneath into the palladium film accumulates, which makes it possible to measure even extremely low release rates that were not accessible before. However, this only works because the loss of hydrogen from the palladium film is negligible. It is unclear why desorption of hydrogen from the palladium film is so surprisingly low. It is assumed that the ultra-thin water layer remaining at room temperature on the surface even under the dry nitrogen gas atmosphere that is used for the measurements, plays an important role in inhibiting desorption. In order to obtain a better understanding of this (and because this could also help with our understanding of electrochemical reaction at buried interfaces) a novel focus of research within the group is the fundamental investigation of electrochemical double layers and how their structure affects the kinetics of reactions such as oxygen reduction. For this purpose a novel lab environment with a newly acquired Near Ambient Pressure – X-ray Photolectron Spectroscopy NAP-XPS has been built up. The research in this new laboratory is partly closely related to the excellence cluster RESOLV.

3. Measurements of Hydrogen distribution and effect on embrittlement
The novel SKP and SKPFM based method for hydrogen mapping that was developed with the Christian Doppler Laboratory is now becoming a central tool of research on hydrogen related topics, in close cooperation with other departments (see p. 39).

4. Semiconducting properties of surface oxide films
An especially important topic are novel Zinc-Aluminum-Magnesium alloys (ZAMs) where in earlier works the native oxide layer was shown to play a crucial role in the delamination behaviour. For blank corrosion, the properties of the corrosion product layers that grow during exposure are widely assumed to determine the corrosion performance. In many corrosion tests especially the presence of magnesium in the alloys is found to provide significantly enhanced corrosion behaviour, but only under certain environmental conditions [13-16]. The novel Fe-Zn-Mg alloys that are currently being developed for application on steel parts that will undergo hot stamping will have to be investigated in terms of their oxide properties, too.

5. Intelligent self-healing concepts for corrosion protection
After successful finishing of the MPG-FHG co-operative project on active corrosion protection (ASKORR) the main activities on self-healing are currently carried out within the framework of the DFG SPP “Self-Healing Materials” Within the reporting period we succeeded to synergistically combine capsule loaded zinc coatings with capsule loaded organic coatings for superior intelligent self-healing [39]. Other important results were the development of polyaniline PANI based capsules for intelligent release and their modification for use on zinc and first successful application of intelligent corrosion protection [37-38]. Of special importance is the interfacial stability between conducting polymer and the metal surface [104-105]. Furthermore, a novel strategy for addressing also capsules located deep in the organic coating far away from the metal surface was developed by additionally adding non redox active conducting particles, such as carbon black [106]. The current main activity is to investigate how the coating design has to be modified in order to be able to routinely self-heal defects of macroscopic size, such as 1-2 mm broad scratches, with coatings just a 10-20 microns thick. For this, the propagation of the trigger signal for initiating the release at the onset of corrosion in a defect site has to be very fast and it has to be able to travel deep into the coating. Also release and transport of the active agents from the capsules in the coating to the defect site has to be fast and it is necessary to activate as much of the stored compounds for self-healing as possible. This requires a totally new philosophy for coating design.

6. Novel developments with the Scanning Kelvin Probe
A technique of central importance for many research projects within the group is the Scanning Kelvin Probe technique. Based on our world leading expertise of this technique also novel application fields are explored. The recent development of spatially resolved high-sensitivity hydrogen detection by Kelvin probe (see Christian Doppler Laboratory and p. 39) has sparked new research on the possibilities to further extent the applicability of the Kelvin probe. In cooperation with Christian Michelsen Research a novel Kelvin probe for outdoor use and for through metal corrosion detection (signal mediated by hydrogen activity at the corroding defect and its permeation through the metal) is currently being developed.

Another development is the use of Kelvin probe for assessing oxygen reduction rates at buried interfaces. Also for the investigation of tunnelling junction in molecular electronics the technique was successfully applied [108], as well as for investigation of lipid layers [109].

Interaction Forces and Functional Materials (M. Valtiner)

The research interest of the Interaction Forces group is focused on the broad areas of adhesion in wet environments, molecular structuring at solid/liquid interfaces, reactivity in confinement and high resolution imaging and detection of corrosive processes. The broader scientific aims are (1) to gain insight into the molecular interactions at equilibrated and dynamically changing reactive interfaces. Also, it is studied (2) how molecular interactions translate into macroscopic interactions (scaling and proportionality laws), and (3) new interferometry-based approaches to study dynamic processes *in-situ* are developed. A particular focus is on how molecular structuring at electrified interfaces influences the mentioned processes. In detail the following scientific topics are of current interest:

1. Molecular scaling and proportionality laws at adhesive interfaces over large length scales
   As already mentioned above a unique experimental framework to test the well-renowned Jarzynski's equality was developed, which relates work performed under non-equilibrium conditions. Based on this we developed a scaling strategy that allows us to predict large-scale properties such as adhesion at electrified interfaces on the basis of single-molecule measurements [36].

2. Fundamentals of peptide materials (Collaboration with UC-Santa Barbara)
   In a **joint project with our collaborator Prof. M.S. Shell from UC Santa Barbara, U.S.A.** state-of-the-art **single molecule atomic force microscopy (SM-AFM) hand-in-hand with advanced molecular simulation** studies were combined to obtain innovative fundamental insights into peptide materials, their self-assembly properties, and their ability to mediate interactions at solid/liquid interfaces. Materials made from peptides are becoming of widespread importance for their tunability, biocompatibility, and sustainability & environmental friendliness. Designer self-assembled peptides form a myriad of nanostructures and have been used as materials for tissue engineering and recovery, drug delivery, biosensing, and inorganic templates and scaffolds. Peptides also offer powerful routes to modify interactions at solid interfaces. They readily tune surface properties (from antibacterial to ultra-hydrophobic moieties), and potentially provide platforms for tissue gluing and environmentally friendly adhesives, based on biomimetic concepts.

   Marine animals such as mussels and barnacles e.g. use an optimized hierarchical structure and a large variety of functional peptides sequences in order to achieve unprecedented adhesion in high salt concentration environments. Here, even on a molecular scale the arrangement of individual bonds massively influences adhesive strength. As anticipated adhesive strength increases with an increasing number of bonds in parallel while an increasing number of bonds in series reduces the strength of an adhesive junction. We recently showed how adhesion forces could be manipulated by the number of interacting bonds in parallel and in series using designer peptides [110]. It was shown how the arrangement of individual bonds in an adhesive junction allows a tuning of adhesive strength even without changing the underlying adhesive bond. Further our unique AFM approach allows us to directly measure interaction free energies of peptides with various surfaces [35]. Based on this experimental data simulation probes can be both tested and finally utilized to provide a full molecular level understanding of interactions of peptides with surfaces in aqueous environments. Finally combination of both AFM single molecule force spectroscopy data and Molecular Dynamics MD-simulations is planned, in order to bridge experiment and theory at the solid/liquid interface.

3. Electrochemistry in confined spaces
   Our unique electrochemical surface forces apparatus allows us to utilize white light interferometry (WLI) to directly visualize corrosion processes in real-time, *in-situ* in confined (i.e. buried) geometries [111]. This is a unique experiment that allows to *in situ* study crevice corrosion with unprecedented resolution in time and space. In a first case study, we investigated in detail how pure **aluminum corrodes in crevice geometries and how vanadate ions can effectively inhibit CC of aluminum** (Fig. 2). We are now continuing into this direction and study how various inhibitors also influence crevice corrosion on real alloy samples. For this we are currently constructing a back-scattering version of the EC-SFA.

4. Electric double layers in static and dynamically changing systems (Collaboration with the cluster of excellence – RESOLV at the Ruhr University Bochum). The molecular structure of the electric double layer is essential in electrochemical and natural processes. In particular, ion and water structuring at charged solid/electrolyte interfaces dominate structure and functionality in many

physiological, geological, and technological systems. In technological concentration ranges above 50-100 mM concentrations electrolyte structuring occurs within the range of molecular dimensions. Yet no qualitative or quantitative model exists for predicting ion structuring at solid/liquid interfaces. In collaboration with the Cluster of Excellence RESOLV (see p. 54), we started to use force probe experiments as workhorse to directly probe structural forces at solid7liquid interfaces. For instance we showed how specific ion adsorption can strongly influence how electric charge is compensated in the electric double layer on model ceramic surfaces [113].

5. Influence of trace molecules on structuring of ionic liquids at electrified and charged interfaces
Within the last years we utilized **force probe experiments and XPS measurements** to directly measure how water and other impurities alter the interfacial structuring and charging characteristics of RTILs on dielectric surfaces and electrified metal surfaces [113]. On ceramic interfaces water can dissolve surface-bound cations, which leads to high surface charging and strong RTIL layering. In contrast, layering of dry RTIL at weakly charged mica surfaces is weakly structured. At electrified gold electrodes the influence of water is limited to interactions within the RTIL layers, and is not related to a direct electrosorption of water on the polarized electrode. Currently, we are testing the influence of other potentially beneficial additives such as organic long-chained molecules and polymer materials. Generating such detailed insights into molecular interface structures will further guide the targeted development of structures at electrified interfaces.

6. High resolution imaging of active corrosion (Collaboration with Hasselt University)
Together **with our collaborator F.U. Renner from Hasselt University, Belgium, we recently performed a high-resolution *in-situ* atomic force microscopy study of dealloying of Cu–Au alloy surfaces** [115]. It was found that dealloying patterns, and in particular crack initiation are highly influenced and controlled by the choice of inhibitor molecules, and is also affected by larger scale structural defects such as scratches or polishing defects [115] as well as crystallographic surface orientations.

   In this direction we specifically studied how surface cracks formed during local dealloying of Cu_3Au. Crack induction clearly depends on the crystallographic substrate orientation, which is controlling the number density of cracks on each grain [116]. The highest number density was observed on (110) oriented surfaces and the lowest on (001) and (111) grains.

7. Combining electrochemical force probe experiments with optical spectroscopy.
The technological focus of the group is the design of novel experiments and experimental setups dedicated to understand interfacial dynamics such as specific and non-specific binding and unbinding events at electrified interfaces. Coupling of laser light into our force probe experiments has been successfully realized and implementation of Raman spectroscopy into the electrochemical Surface Forces Apparatus is the next aim, in close collaboration with the Optical Spectroscopy group of Andreas Erbe.

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Research Projects in Progress

Electrocatalysis

Baldizzone: Degradation of carbon-supported Pt bimetallic nanoparticles

Cherevko, Zeradjanin, Grote: High-throughput material screening for electrochemical CO_2 reduction

Grote, Zeradjanin, Cherevko: CO_2 reduction product analysis by SFC coupled with DEMS

Cherevko, Kasian: Mechanism of metal oxide dissolution in acidic media

Geiger: Investigation of high-surface area catalysts for OER

Kasian, Cherevko, Geiger, Ludwig: Investigation of material libraries based on nobel metal oxides

Zeradjanin: Key denominators for HER/HOR

Kulyk: Modelling of mass transport and cell geometry impacts on electrochemical reactions

Keeley: Particle-size effects on dissolution of noble metals

Hodnik: Development of electrochemical *in-situ* electron microscopy

Pizzutilo: Oxygen reduction reaction on noble metal catalysts

Pizzutilo: Hydrogen peroxide production on AuPd alloys

Polymeros, Baldizzone: Study of fuel cell catalyst stability under simulated start up/ shut down conditions

Polymeros: Development of an advanced characterization tool for high-surface area catalysts

Hodnik, Baldizzone: Influence of thermal pre-treatment of fuel cell catalysts on durability

Baldizzone, Pizzutilo, Schüth: Influence of catalyst support on activity and stability - hollow graphitic sphere based platinum nanoparticles

Rossrucker: High throughput screening of zinc and zinc-magnesium material libraries with a SFC and downstream analytics

Kasian: Stability investigation of Ir and Ir-based alloys utilizing a high-throughput SFC coupled with ICP-MS

Choi: Single atom catalysts for electrochemical reactions

Choi, Grote: Stability of non-noble catalysts for ORR

Interface Spectroscopy

Altin, Rohwerder, Erbe: Cyclodextrines as controlled release systems in corrosion protection

Altin, Krieger, Wohletz, Groche, Springer, Erbe: Corrosion of aluminium-steel joints prepared by cold forging

Chen, Erbe: Step-scan FTIR studies of electrode/electrolyte interfaces

Chen, Toparli, Erbe: Characterisation of organic corrosion inhibitors on copper

Ebbinghaus, Erbe: Visualisation of delamination by infrared microscopy

Fernandez Solis, Rohwerder, Erbe: Coatings based on water-soluble biopolymers

Genchev, Todorova, Springer, Erbe: Corrosion of iron-based alloys in H_2S-containing media

Ksiazkiewicz, Fernandez Solis, Erbe: Characterisation of oxidation products of biopolymer films on zinc

Mondragon Ochoa, Rohwerder, Erbe: Synthesis and electrochemical characterisation of well-defined thin model polymers by atomic transfer radical polymerisation

Niu, Schulz, Schmid, Erbe: Analysis of electrode potential dependent water structure at the germanium/electrolyte interface by attenuated total reflection infrared spectroscopy

Pander, Tecklenburg, Yang, Wippermann, Erbe: Stabilisation of the silicon/electrolyte interface for infrared spectroscopic investigations

Rabe, Erbe: Mechanistic investigations of the oxygen evolution reaction on manganese electrodes

Rechmann, Götzinger, Dirksen, Müller, Erbe: Electrochemical properties of phenothiazine-modified metal surfaces

Sarfraz, Toparli, Zeredjanin, Erbe: Investigation of oxide growth at the platinum/electrolyte interface

Schwenzfeier, Hu, Valtiner, Erbe: Development of a matrix method based analysis scheme for interferometric spectra recorded in the surface force aperatus

Tecklenburg, O'Donoghue, Devi, Erbe: Preparation of atomically defined ZnO films and spectroscopic characterisation of its interaction with water

Toparli, Sarfraz, Erbe: Investigation of electrode surfaces in the transpassive regime by *in situ* spectroscopies

Corrosion

Altin, Rohwerder, Erbe: Cyclodextrines as controlled release systems in corrosion protection

Bashir, Rohwerder: STM, SKPFM and SKP for surface characterisation

Merzlikin, Rohwerder: TDS characterisation of hydrogen in steels

Tran, Rohwerder: intelligent corrosion protection by nanocapsules incorporated to the zinc coating: understanding co-deposition and synergy with organic coating

Evers, Bashir, Rohwerder: spatially resolved and ultra-sensitive hydrogen detection in steels and investigation of hydrogen uptake

Bashir, Rohwerder: SKPFM for the investigation of hydrogen in metals: further developing the technique

Merzlikin, Rohwerder: Novel corrosion protection coatings for hot forming

Merzlikin, Tran, Rohwerder: Guidelines for use of welded stainless steel in corrosive environments

NN, Rohwerder: Role of microstructure in zinc alloy coatings on corrosion performance

Evers, Rohwerder: Investigation of the potential use of Kelvin Probe for detection of corrosion at the inside of tank and pipeline walls

Evers, Rohwerder: Investigation of the potential use of Kelvin Probe for detection of corrosion under extreme conditions

Merz, Rohwerder: Investigation of optimal distribution of conducting polymer within an organic coating and at the interface with the metal for achieving optimal corrosion protection

Uebel, Rohwerder: Fundamental investigation of coating requirements for fast self-healing of large defect sites in organic coatings

Krieger, Merzlikin, Rohwerder: Role of hydrogen activity on trapping at internal oxides

Krieger, Merzlikin, Springer, Rohwerder: Fundamental investigation of role of microstructure on hydrogen embrittlement

Dandapani, Rohwerder: Investigation of oxygen reduction at the interface between metal and organic coating by use of a novel permeation based technique

Kerger, Rohwerder: In-situ investigation of electrochemical oxygen reduction and metal oxidation by ambient ESCA

Beibei Peng: Fundamental investigation of the emersed electrochemical double layer

Wengert, Vogel, Vogel, Rohwerder: investigation of oxygen uptake and its effect on short term internal oxidation

Wu, NN, Rohwerder: Characterization of hydrogen trapping sites in steels at high spatial resolution by means of SKPFM and permeation techniques

Interaction Forces and Functional Materials

Utzig, Stock, Raman, Valtiner: Fundamentals of Peptide Materials

Cheng, Hu, Merola, Baimpos, Valtiner: Electric double layer structures in highly concentrated electrolytes and ionic liquids

Hu, Shrestha, Valtiner: Electrolyte structuring and electric double layers at static and dynamic electrified interfaces

Merola, Hu, Cheng, Shrestha: Corrosion in confinement (Crevice corrosion and stress corrosion cracking)

Merola, Valtiner: Conductivity in ultra-thin surface films (oxides and organic barrier layers).

Buvaneswaran, Gonzalez, Valtiner: Scientific programming of machine controls and feedback mechanism for force spectroscopy and surface forces apparatus.

Buvaneswaran, Valtiner: Design of novel force probe techniques for measuring equilibrated single molecule force distance spectra

Schwenzfeier, Hu, Valtiner, Erbe: Development of a matrix method based analysis scheme for interferometric spectra recorded in the surface force aperatus

Hu, Valtiner: Hydration lubrication, friction and damage in tribological and tribocorroding systems in aqueous solutions.

Cheng, Valtiner: Wetting of nano-confined spaces by battery electrolytes

Baimpos, Valtiner: High-resolution *in-situ* study of the swelling/shrinkage of Metal-Organic-Frameworks during loading/unloading with gas molecules

Raman, Stock, Valtiner: Design, synthesis and testing of novel adhesion promoting bio-molecules for superior wet-adhesion

Stock, Utzig, Valtiner: Hydrophobic interactions at the macroscopic and single molecular scale

Stock, Müller, Valtiner: Influence of specifically adsorbing ions on hydrophobic interactions

Raman, Stock, Utzig, Moreno-Ostertag, Valtiner: Single molecule physics at electrified interfaces

Chen, Valtiner: Preparation and manufacturing of dielectric mirrors for interferometry applications

Atomistic Modelling

Scalise, Wippermann: Nanointerfaces in InAs-Sn_2S_6 nanocrystal-ligand networks

Nugraha, Wippermann: 3C-SiC/SiO_2 interfaces in SiC nanofiber-based solar cells: characterization from joint *ab initio* thermodynamics and electron paramagnetic resonance simulations

Yang, Tecklenburg, Wippermann, Erbe: Joint first principles and ATR-IR study of the vibrational properties of interfacial water at Si:H-H_2O solid-liquid interfaces

Kenmoe, Biedermann, Wippermann, Todorova, Neugebauer: Stability and vibrational properties of water thin films on low index ZnO surfaces

Vatti, Yang, Wippermann, Todorova, Neugebauer: Ion solvation energies and solvation shell vibrational dynamics

Biedermann, Todorova, Neugebauer, Wippermann: Surface phase stability at Ge-water interfaces from *ab initio* molecular dynamics

Wippermann: First Principles Kelvin probe force microscopy study of stepped Silicon surfaces

Wippermann: Electron-phonon coupling and impurity mediated charge density wave formation in an atomic layer electronic crystal

Wippermann: Non-thermal metal insulator transition in In/Si(111) nanowires

Wippermann: Surface vibrational Raman modes of atomic-scale one-dimensional metallic nanowires

Department of Microstructure Physics and Alloy Design

D. Raabe

Scientific Concept

The department conducts basic research on the relationship between **synthesis, processing, microstructure and properties** of compositionally and structurally **complex materials**. Emphasis lies on nanostructured alloys based on iron, magnesium, titanium, nickel, intermetallics and metal-matrix composites which are characterized by a large variety of **phase transformations**, **kinetics** and **defect substructures**. We apply **advanced characterization** methods from the single atom level up to the macroscopic scale together with **multiscale simulation** methods, focusing on mechanical structure-property relations. Our preferred experimental tools are local electrode atom probe tomography (APT) correlated with transmission electron microscopy (TEM) [1-20], cross-correlation EBSD (electron backscatter diffraction) and 3D EBSD methods [21-24], electron chaneling contrast imaging (ECCI) under controlled diffraction conditions [25-34], and *in-situ* micromechanical experiments correlated to local strain mapping and micromechanical simulations [35-41]. Our modeling tools have been rendered into the modular **freeware simulation package DAMASK** (Düsseldorf Advanced Material Simulation Kit) which is a hierarchically structured model of material point behaviour for the solution of elastoplastic boundary value problems along with damage and thermal effects [42-54]. Our approaches and main topics are shown in Fig. 1. Some of the most exiting scientific fields currently pursued are shown in Fig. 2.

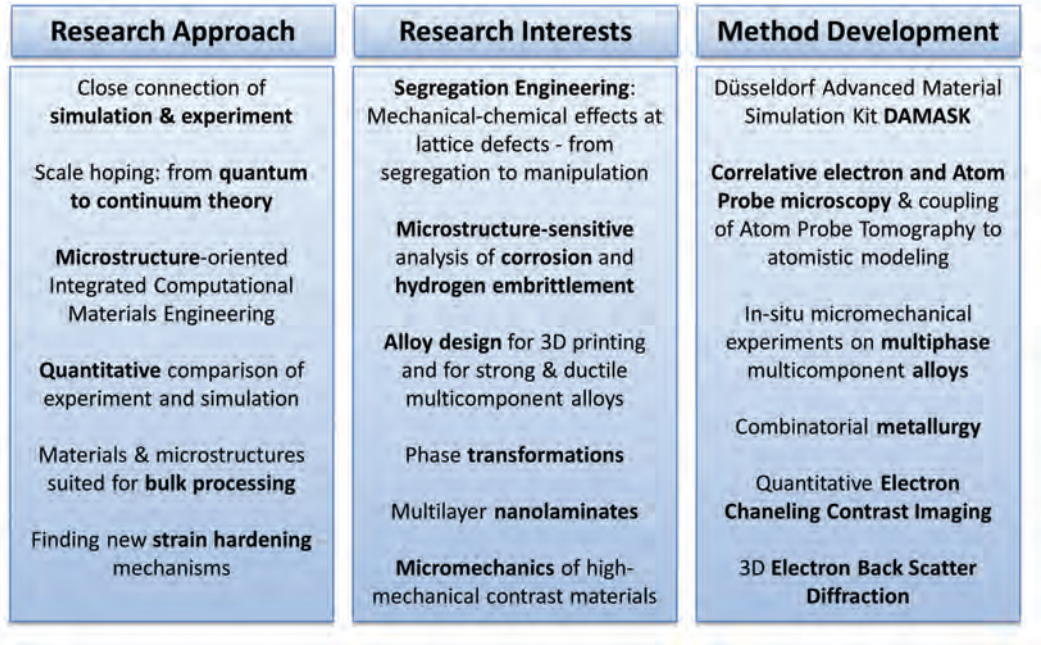

Fig. 1: *Research approach, interests and corresponding long-term method development in the Department for Microstructure Physics and Alloy Design.*

Research Groups

The department is organized in scientific groups some of which are extramurally funded and hence non-permanent, Fig. 3.

The group '**Theory and Simulation**' of Franz Roters develops mechanism-based constitutive models [55-57] for steels, Ti and Mg alloys, focusing on crystal plasticity approaches [29,35,36,42-54]. Models range from phenomenological descriptions to physics-based formulations of **dislocation** slip, **twin-**

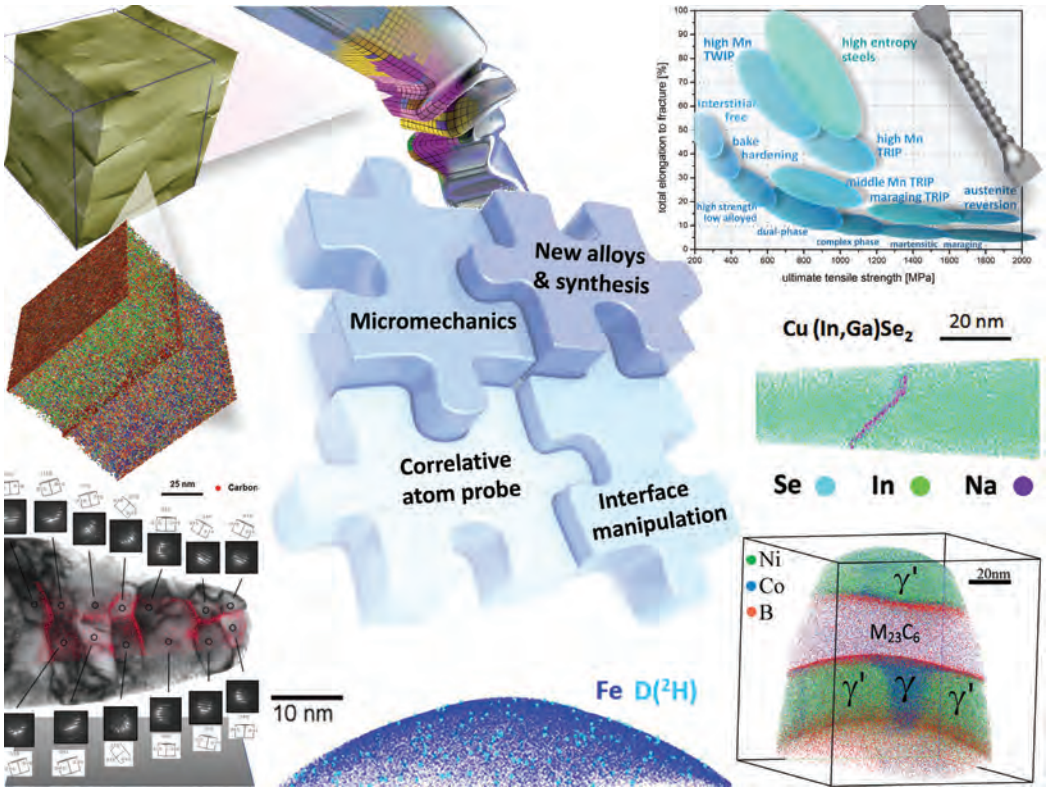

Fig. 2: *Some scientific fields currently pursued in the Department for Microstructure Physics and Alloy Design.*

ning induced plasticity (TWIP) and **martensitic transformations** (TRIP) [29]. The mean field models describe the evolution of lattice defects such as dislocations and twins under given mechanical or thermal boundary conditions. The predicted defect densities enter into kinetic structure-property relations that translate them into strength and deformation measures [55-57]. Owing to the crystalline anisotropy of metallic alloys the constitutive laws assume a tensorial form, i.e. they predict the defect evolutions on all crystallographic shear and twinning systems and their interactions. The resulting sets of nonlinear internal-variable differential equations are solved using either the **Finite Element Method** (CPFEM) or a **Spectral Method** (CPFFT) [58-60]. The models are accessible through the modular simulation framework DAMASK (*http://damask.mpie.de*) [42] (see p. 45).

The group '**Microscopy and Diffraction**' of Stefan Zaefferer pursues two correlated tasks: on the one hand, its projects aim at understanding microstructure formation mechanisms and the relation between microstructures and properties of materials by investigations at the microscopic level. To this aim, several SEM-based microscopy and **electron diffraction techniques** (EBSD, 3D EBSD, XR (cross-correlation)-EBSD, ECCI) have been developed and advanced [21-35]. Imaging and diffraction in transmission electron microscopy (TEM) and x-ray diffraction is conducted as well. With respect to microstructures the focus is on deformation, recrystallization and phase transformations. Concerning properties, corrosion, mechanical behaviour and electronic properties are studied. The spectrum of materials comprises DP (dual phase) steels, TRIP steels, complex phase steels, quench and partitioning steels, electrical steels, austenitic steels, superalloys, Mg-, Al- and Cu alloys, intermetallic compounds and photovoltaic materials [61-64]. The group operates several instruments, e.g. a Zeiss Crossbeam XB1560 FIB-SEM for **3D EBSD** investigations, a JEOL JSM 6500 F SEM, and a JEOL JSM 840A SEM. These instruments are equipped with EBSD, *in-situ* deformation and heating tools. For TEM a Phillips CM 20 is used. This instrument is equipped with the software **TOCA** for on-line crystallographic analysis. Furthermore, several XRD (x-ray diffraction) goniometers are operated.

The group '**Alloy Design and Thermomechanical Processing**' of Dirk Ponge works on the microstructure-oriented **design of advanced high strength steels** and Ni- and Ti-alloys [65-72]. Projects focus on strain hardening mechanisms in complex engineering alloys, making use of processing, mechanical testing and microstructure characterization down to the atomic scale [1,2,73,74]. Thermomechanical processing is a main objective in optimizing steel microstructures and mechanical properties. Main examples are the design of ultrafine grained C-Mn steels and **dual phase (DP)**

Fig. 3: *Research groups in the Department of Microstructure Physics and Alloy Design.*

steels for automotive applications [75]. Recent projects pursue mechanism-based alloy design strategies [70,72]. The joint design of **novel alloys** using **thermodynamic** and **kinetic predictions** in conjunction with **thermomechanical processing** hence describes the current strategy. A recent field of attention was the analysis of Mn-based model steels [1,14]. Mn is an important alloying element for tuning austenite stability, stacking fault energy, and transformation kinetics. While these effects are exploited particularly in designing steels with **TRIP** and **TWIP** effects, novel alloy concepts introduced by the group combine **martensite-to-austenite reversion** with the TRIP and/or **maraging** effects (maraging: martensite aging) [65,74]. Projects in this field have recently also lead to the discovery of the reason for Mn-related **temper embrittlement** [14] and **confined transformation** effects at lattice defects [1].

The group '**Combinatorial Metallurgy and Processing**' of Hauke Springer designs advanced structural materials along with suited synthesis and processing routes and techniques. The focus lies on steels with superior physical and mechanical properties. Projects explore novel pathways for the compositional and thermo-mechanical **high-throughput** bulk **combinatorial** investigation of structural alloy systems [76-142]. Innovative methods for the **accelerated synthesis**, processing and testing of bulk metallic structural materials are developed and applied, so that the associated metallurgical questions (e.g. alloy- and processing-sensitive changes in strain hardening) and corresponding engineering issues (e.g. texture or joining) can be addressed more efficiently over a wide composition and processing range. Such methods are referred to as '**Rapid Alloy Prototyping**' (RAP) [76]. This approach refers to semi-continuous high-throughput bulk casting, rolling, heat treatment and sample preparation, and currently allows for the evaluation of the mechanical and microstructural properties of up to 50 material conditions (i.e. five different alloy compositions with ten different thermomechanical treatments each) within a few days. This results in a **rapid maturation** of materials and exploration of bulk material libraries for structural materials under consideration of composition and processing. Research fields addressed by this approach are the *in-situ* synthesis of metal matrix steel composites with high stiffness, martensite-to-austenite reversion steels, lightweight Triplex steels [76,83], the development of high strength steels with inherent weldability and methods for optimised microstructure design by the creation of local chemical gradients which are referred to as **vessel microstructure** steels [82].

The group '**Atom Probe Tomography**' of Pyuck-Pa Choi explores compositionally complex structural and functional materials based on the atomic scale information obtained with Atom Probe Tomography (APT) [1-20]. The group was supported by funds from the **Leibniz Award.** It operates two local electrode APT instruments (LEAP 3000X HR, LEAP 5000XS). APT is a high-resolution characterization technique for 3D elemental mapping with near-atomic resolution. It is used for studying nanoscale phenomena such as precipitation, solute clustering, segregation at defects, complexions and partitioning effects [1,69]. An important approach towards better understanding of APT data is the correlation between experiment and theory, conducted in collaboration with the department of J. Neugebauer. Current projects are on high-strength alloys such as **high-Mn steels**, Ni- and Co-based **superalloys** as well as **nanostructured** materials such as cold-drawn **pearlitic steel wires** and **sputter-deposited thin-film multilayers** [1-20,90-111]. Functional materials under investigation are Fe- and Co-based metallic glasses for **magnetic applications**. The group also studies **semiconductors** for **photovoltaic** applications in close collaboration with the group of O. Cojocaru-Mirédin (Interface Design in Solar Cells) [90-93]. Special attention is placed on **correlative TEM and APT** for the joint structural and chemical analysis of atomic-scale microstructure features.

The new group on '**Alloys for Additive Manufacturing**' of Eric Jägle was established in 2015 [94]. While particularly **Laser Additive Manufacturing** (LAM) is well-established to produce metallic parts, the optimization of alloys and the design of new materials tailored for LAM are still missing. Established alloys currently in use do not exploit the opportunities inherent in this technique, leaving

a gap towards its further development. Funding for the group comes from the joint Max-Planck Society/ Fraunhofer Society research project "AProLAM" - **Advanced Alloys and Process Design for Laser Additive Manufacturing of Metals**. In this project, the two partners Max-Planck-Institut für Eisenforschung (MPIE) and Fraunhofer Institute for Laser Technology (ILT) work together on the development of alloys for the LAM process and at the same time on the adaptation of the LAM process for the synthesis of **new alloys**.

The group for '**Adaptive Structural Materials**' of Cem Tasan develops novel experimental-theoretical tools to understand micro-mechanisms governing macro-properties and design property-optimized novel structural alloys [35-41]. The group is linked to the theory group of B. Grabowski (Department of Computational Materials Design) and sponsored by an **ERC Advanced Co-Investigator Grant** of D. Raabe and J. Neugebauer. Conventional **hardening mechanisms** lead to a decrease in ductility. With the development of **adaptive structural materials** (ASM) the group's key idea is based on designing, synthesizing and characterizing **intrinsic phase instability**. The philosophy behind that is to either incorporate dispersed phases that are close or even beyond their mechanical and thermodynamic **stability limit** into otherwise stable bulk alloys or to design the bulk material itself such that it is at the verge of mechanical/thermodynamic stability. In either case the phases transform under loading into secondary phases (i.e. martensite) or extended defects (e.g. twin bundles). The group combines quantum-mechanically guided design with *in-situ* experimentation. On the theory side, the group of B. Grabowski has developed approaches to accurately describe finite temperature effects from first principles [37,95-99]. On the experimental side the group employs (i) various metallurgical production and processing routes, (ii) multi-scale characterization down to atomic resolution and mechanical testing, and (iii) high-resolution *in-situ* characterization of phase transformations and deformation mechanisms [72,145]. The latter is of particular importance for ASMs, since the determination of the stable regimes of the introduced unstable phases is in most cases only possible through such *in-situ* analysis. The group leader Cem Tasan has accepted a **faculty position at MIT** in Cambridge, USA, starting January

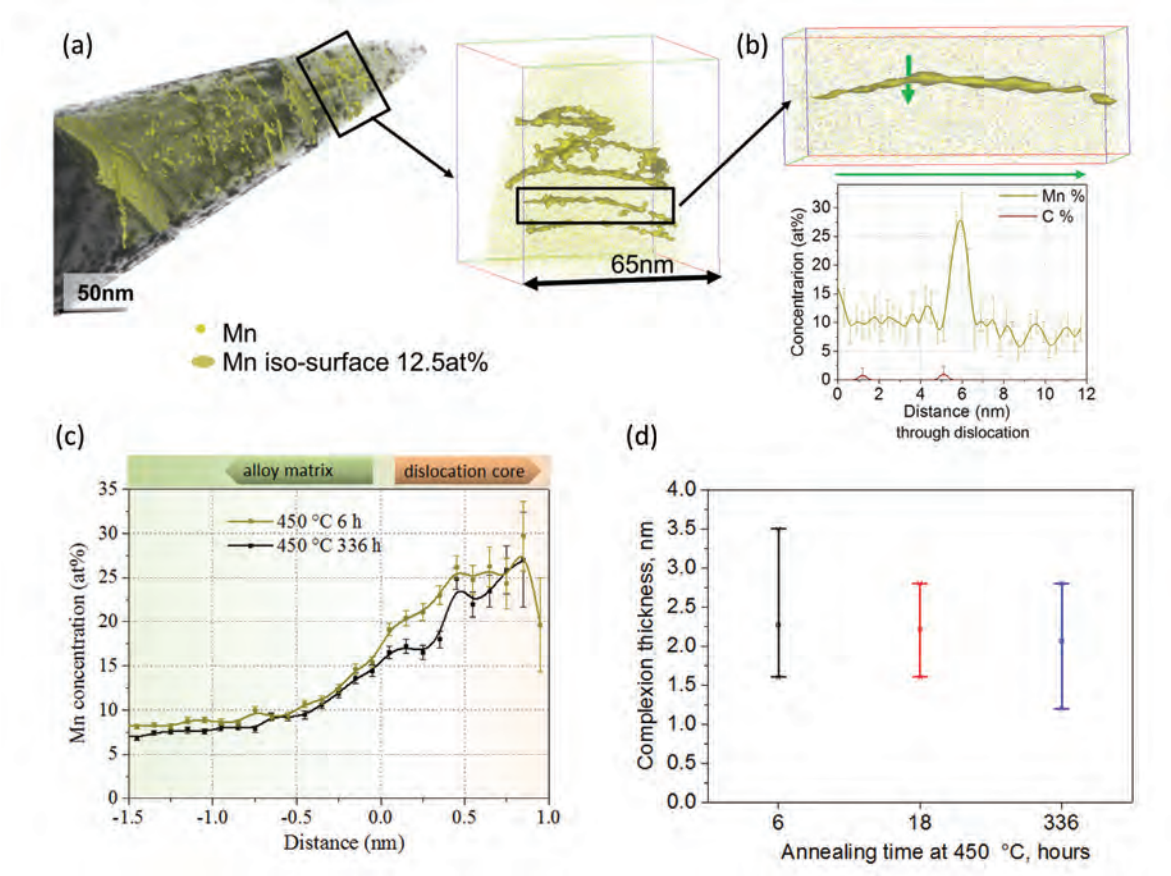

Fig. 4: *Fe-9 at. % Mn solid solution, 50% cold-rolled and annealed at 450°C for 6 hours to trigger Mn segregation [1]. (a) Correlative TEM - APT. (b) Subregion and 1D compositional profile along the dislocation line. (c) Proximity histograms. (d) Prolonged aging neither affects size nor composition of the austenitic dislocation core regions which is one of the most characteristic features of linear complexions.*

2016. The work will in future be pursued in close collaboration with his group at MIT.

The group '**Interface Design in Solar Cells**' of Oana Cojocaru-Mirédin aims to understand the relationship between the chemical, electrical, and structural properties of interface-dominated solar cells. Focus is placed on **multicrystalline silicon** (m-Si) solar cells, and $Cu_2ZnSnSe_4$ (CZTS) and $Cu(In,Ga)Se_2$ (CIGS) **thin-film solar cells** because of their relatively **high efficiency**. To better understand these materials the group performs correlative studies on specific regions using joint EBSD / TEM, electron beam-induced current (**EBIC**)/ **cathodoluminescence**, and **APT** [90-93]. The mission is to optimize solar cell efficiency based on the 3D chemical analysis at the atomic-scale. The atomic redistribution of the impurities at the internal interfaces (grain boundaries and p-n junction) may affect the efficiency of a solar cell. For example, the efficiency of a CIGS solar cell has been improved by almost 50% only by Na doping (~ 0.1 at.%) inside the absorber layer. Furthermore, it was observed that this increase in the efficiency can be directly correlated with the Na segregation at the CIGS grain-boundaries. The group is financed by the federal ministry "Bundesministerium für Bildung und Forschung" (NanoMatFutur competition). The group leader Oana Cojocaru-Mirédin has recently accepted a permanent group leader position at RWTH Aachen. Corresponding topics will in future be pursued in close collaboration.

The group '**Biological Composites**' of Helge Fabritius works on the interactions of structure, composition and properties of **biological materials**. The group was established in 2008 from funds of the **Leibniz Award**. Projects aim to reveal how nature designs and optimizes materials through modifications in structure and composition from the molecular level up to **specialized tissues** and functional parts. The group pursues an integrative approach combining **experiments and simulations** based on detailed structural characterization [100-108]. Recently, the group works on the development of **bio-inspired and biomimetic** materials such as **optical sensors** [102] and **dental materials** [100,103]. The main model material in the group is the Arthropod cuticle [101]. Its structure consists of fibrillary chitin and proteins independent of the exact location. Owing to its double function as integument and exoskeleton, the cuticle fulfils different functions that require a variety of physical properties. These can be mechanical, optical, and also combinations of several properties within the same skeletal element such as the transitions between the elastic arthrodial membranes and the rigid mineralized cuticle of limb segments. Other model materials include vertebrate **bones** and **teeth**, specifically those of sharks [100,103,105].

Main Research Interests

The objectives of the research groups and their core competences were described above. Here we present our **recent progress** in a number of **key interdisciplinary areas of interests** in the department which are **jointly pursued** by members of different groups including also members from other departments. More specific **scientific details** about some of these projects are given in the section **"Interdepartmental Research Activities - Selected Highlights".**

Segregation Engineering: Mechanical-chemical effects at lattice defects - from segregation to manipulation

Dislocations and **interfaces** influence mechanical, functional, and kinetic properties of alloys. They can be manipulated via **solute decoration** enabling changes in energy, mobility, structure, and cohesion or even promoting local phase transformation. In the approach which we refer to as **'segregation engineering**' solute decoration is not regarded as an undesired phenomenon but is instead utilized to manipulate specific defect structures, compositions and properties [1,14,69,74].

For instance we found that **grain boundary (GB) segregation engineering** and local austenite reversion can turn interface embrittlement into toughness [14]. In a Fe-9 wt.% Mn martensite we studied **grain boundary embrittlement** in the quenched and tempered state. While solute Mn directly embrittles martensite grain boundaries, reversion of martensite back to austenite at grain boundaries cleans the interfaces from solute Mn by partitioning the Mn into the newly formed austenite, hence restoring **impact toughness** (see p. 50; see p. 173).

Fig. 4 shows the discovery of a chemical and structural state confined to dislocation cores which we refer to as **linear complexion** [1]. Dislocations attract solutes according to the Gibbs isotherm. The concept of interface complexions extends the classical isotherm to **interface-stabilized states** that have a structure and composition different from that of the matrix and remain confined in the region where they form. We observed such a phenomenon at edge dislocations in a binary Fe-9 at.% Mn alloy in which a stable confined austenite structure forms in an otherwise martensitic crystal. This is a 1D analog of the previously observed **complexions** that were observed at planar defects (see p. 50; see p. 181).

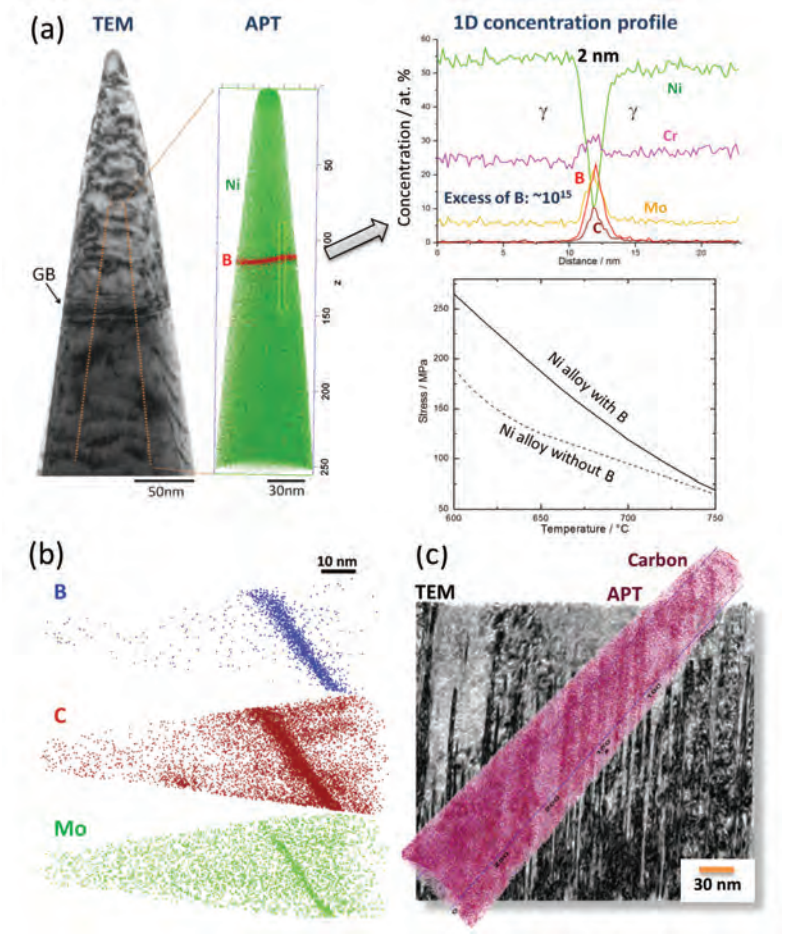

Fig. 5: *Segregation of B to a high angle GB in Ni-alloy 617. B improves - via improved GB cohesion and GB precipitation - the rupture strength as shown in terms of the comparison of alloy 617 (Nicrofer5520Co) and the B-doped variant alloy 617B (Nicrofer5520CoB) in the range between 600 to 750°C (105h) [110]. Segregation of B is also found at prior austenite grain boundaries in quenched martensitic steels [73]. In as-quenched Fe-C martensite the cooling rates are typically too slow to entirely freeze C in at its original positions. Hence, C relaxes to lath interfaces [2].*

Fig. 5 shows examples where I**nterface Segregation Engineering** was used to **enhance grain boundary cohesion**. An example is B doping of creep-resistant polycrystalline **Ni-based alloys** used for power plant applications. Fig. 5 shows alloy 617 where **B segregation** on **grain boundaries** was revealed by using **correlative TEM-APT**, leading to enhanced grain boundary cohesion and the promotion of the formation of precipitates [110]. B segregation was also found at **prior austenite grain boundaries** in quenched **martensite**. In these materials we found that B and Mo segregate only to prior austenite grain boundaries but are absent at martensite–martensite interfaces. C segregated both at prior austenite grain boundaries and at martensite–martensite boundaries. Even in conventional as-quenched **Fe-C martensite** cooling rates are slow enough to allow C relaxation to the lath interfaces.

Microstructure-sensitive analysis of corrosion and hydrogen embrittlement

A main challenge in **corrosion science** consists in identifying the relations between **microstructure features** and the associated electrochemical or physical reactions, respectively, such as **oxidation** [11-115] and **hydrogen embrittlement** [116-121] (see p. 185). In this context, measurements including sufficient spatial resolution of the associated phenomena down to the lattice defect scale are still hard to realize. Yet, the role of individual lattice defects and surface features together with a characterization of their individual structural and chemical state is essential for understanding corrosion and the resulting decay and failure mechanisms. Specifically **site-specific microstructure and composition characterization** is of great relevance. Instrumentation we use in this context are **correlative atom probe tomography**, **Scanning Kelvin Probe** mapping (together with M. Rohwerder) in conjunction with EBSD and ECCI as well as **nanoSIMS** maps. Fig. 6 shows a study on the role of **grain boundaries in the initial oxidation** behaviour of **austenitic stainless steel** at 700°C in air with 20% water vapor for power plant applications [114].

We also compared local hydrogen uptake and release rates by multi-scale **hydrogen mapping** with **spatial resolution** in a Ni-Nb two-phase model alloy, Fig. 7, focusing on two aspects: (1) mapping the **hydrogen distribution** with spatial resolution for establishing the correspondence between desorption profiles and desorption sites, and (2) correlating the obtained results with mechanical testing to reveal the degradation mechanisms. The trapping states were analyzed by **thermal desorption spectroscopy** (TDS). The Ag-decoration method revealed rapid effusion of hydrogen from the matrix, the kinetics of which was spatially resolved through **Scanning Kelvin Probe Force Microscopy** (SKPFM) by the group of M. Rohwerder. The hydrogen release from the matrix steadily decreased until about 100 h and then was taken over by the precipitation phase (δ-Ni_3Nb). The deuterium distribution in the microstructure was studied by **Secondary Ion Mass Spectrometry** (SIMS) (see p. 185).

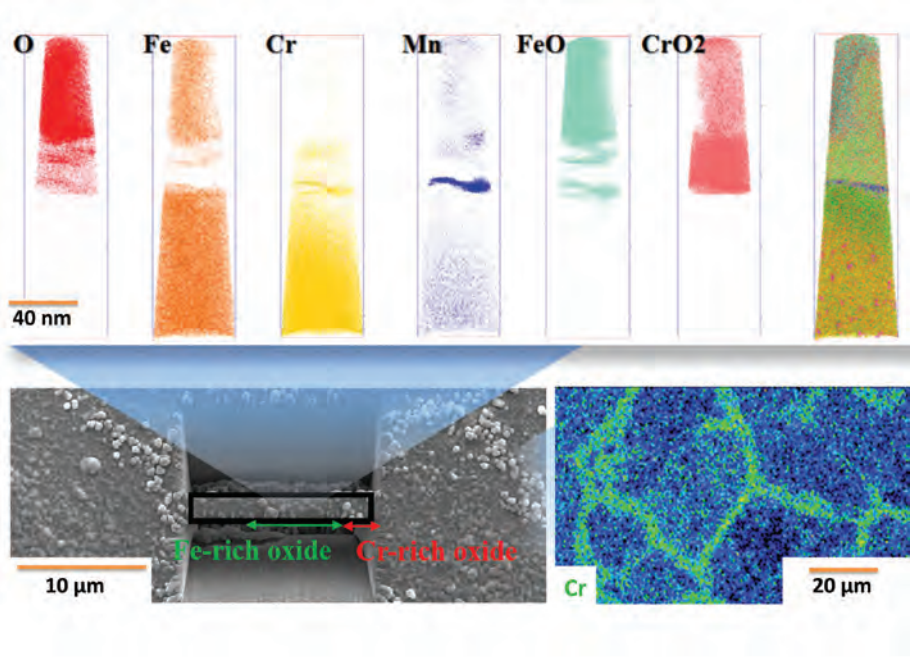

Fig. 6: *Multiscale characterization of microstructure-specific oxidation behaviour (at 700°C) conducted on an austenitic stainless steel [114].*

Fig. 8 shows **hydrogen-induced cracking** at grain and twin boundaries in a Fe-18Mn-1.2C (wt.%) austenitic steel [117-120]. The tensile ductility was drastically reduced by hydrogen charging during tensile testing. The fracture mode was mainly intergranular fracture, though transgranular fracture was also observed. **Transgranular fracture** occurred parallel to the primary and secondary deformation twin boundaries, as confirmed by EBSD and ECCI. The microstructural observations indicated that cracks were initiated at grain boundaries and twin boundaries.

Alloy design for 3D printing and for strong and ductile multicomponent alloys

The **design of novel alloys** is a key challenge for several reasons: First, using thermomechanical processing alone for the design of microstructures is an efficient but limited approach. Including a higher variety of solution and transformation phenomena by **alloy modifications** opens the field of material design beyond the scope offered by processing alone. On the other hand, introducing new compositions without systematic **thermomechanical treatment** studies does also not provide sufficient depth in structural alloy design [122-133]. Hence, we increasingly merge the two disciplines. Second, novel tools such as *ab initio* simulations and kinetic Monte Carlo methods in conjunction with statistical tools such as **ThermoCalc** and **Dictra** render alloy design increasingly accessible to quantitative predictions

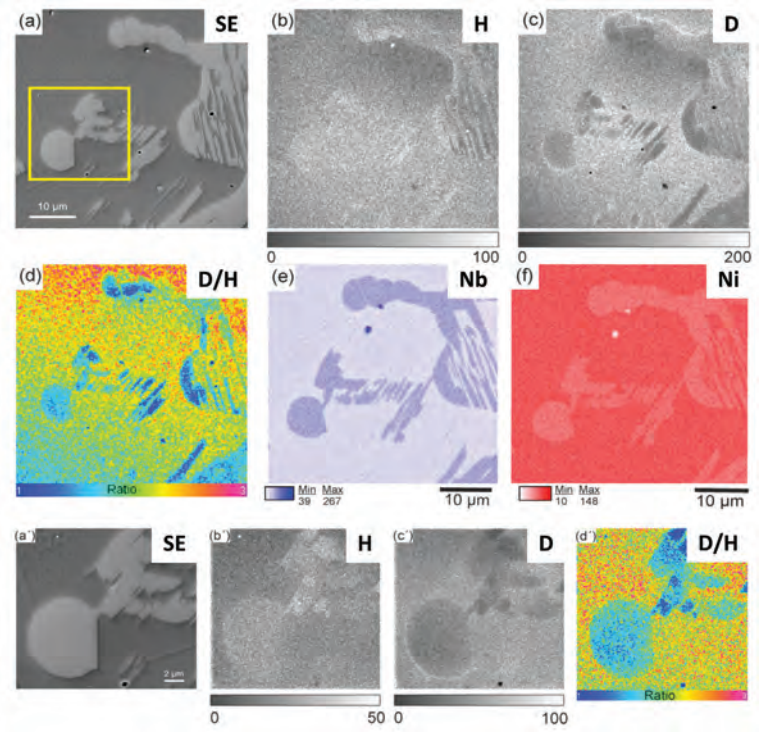

Fig. 7: *NiNb specimen charged with H: (a) SE image and secondary ion maps of (b) H, (c) D, and (d) (2D-/1H-). (e), (f) EDX map of Nb and Ni, respectively. (a´)-(d´) Magnified regions as marked in (a). NanoSIMS in collaboration with L. Yedra and S. Eswara, Luxembourg Institute of Science and Technology.*

[134-138]. Third, high-throughput alloy design methods enable probing wider composition, forming and heat treatment ranges [76-83].

A field of interest for **alloy design** is **Laser Additive Manufacturing** (LAM) [94]. Fig. 9 shows an example where precipitation and austenite reversion in a LAM produced maraging steel were studied. The motivation for this project is that materials produced by selective laser melting (SLM) experience a thermal history that is markedly different from that encountered by conventionally produced materials. In particular, a very high cooling rate from the melt is combined with cyclic reheating upon deposition of subsequent layers. Using APT, we investigated how this thermal history influences the phase-transformation behaviour of LAM synthesized maraging steels (Fe-18Ni-9Co-3.4Mo-1.2Ti) (see p. 25).

We also study **massive solid solution** materials, an alloy class referred to as **high entropy alloys (HEAs)**. We work specifically on materials where the configurational entropy is below its maximum value, Fig. 10 [95,139-144]. The concept was realized in the form of **non-equiatomic multi-component** CoCrFeMnNi alloys produced by rapid alloy prototyping. Their microstructures exhibit a random elemental distribution in a single FCC phase which deforms by planar slip, leading to excellent ductility. We use compositional variations to tune the stacking fault energy and hence the associated transformation phenomena which act as main mechanisms for designing high strain hardening rates (see p. 50).

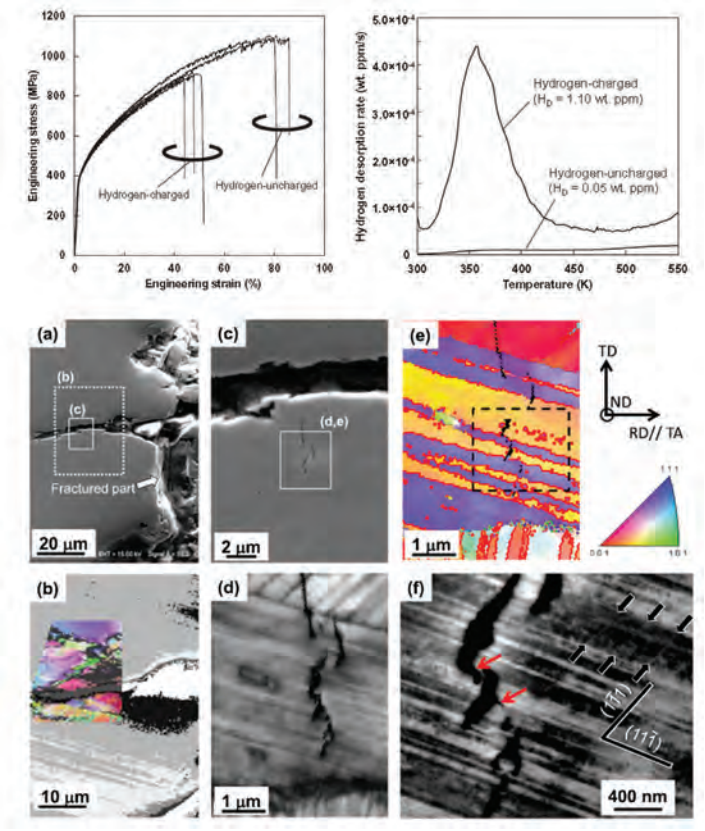

Fig. 8: *Hydrogen embrittlement in an Fe-18Mn-1.2C (wt.%) TWIP steel [119]. Tensile ductility was drastically reduced by H. Top row: Stress–strain curves and H desorption rates in a steel with and without H charging. Bottom images: micrographs near the crack. (a) SEI micrograph. (b) Texture map superimposed on detector signal image. (c) Magnified image of the area within the white lines in (a). (d, e) Image quality and texture maps of area marked by white lines in (c). (f) ECCI corresponding to the area within the black broken lines in (e) [117-120].*

Phase transformations

In conjunction with the **interface segregation engineering** approach discussed above [14,67,109] we developed a class of novel steels which we refer to

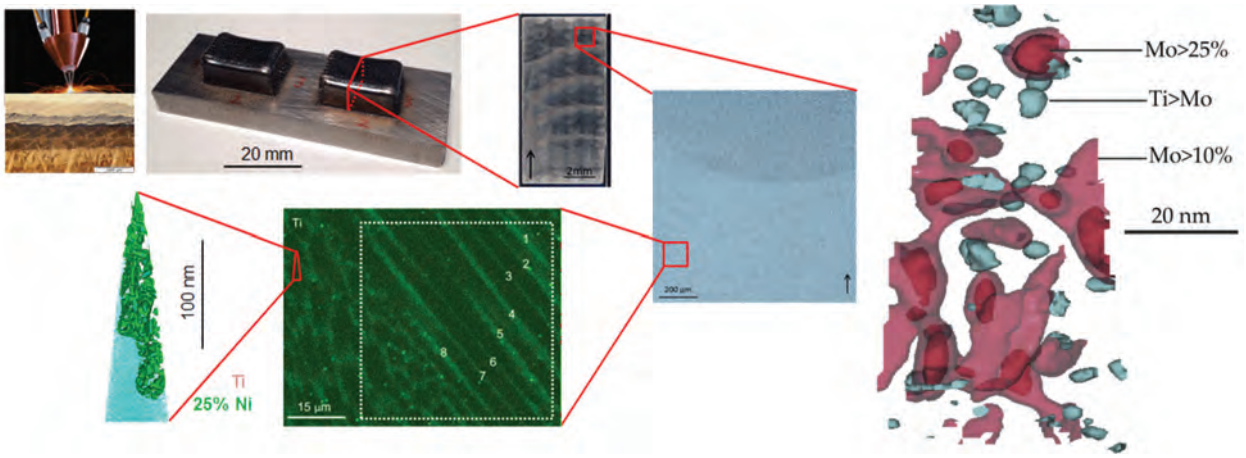

Fig. 9: *Multiscale structural and chemical analysis of maraging steel microstructures obtained from Laser Additive Manufacturing. The APT data set on the right hand side provides three isoconcentration surfaces for identifying the stoichiometry of the different nanoprecipitates [94].*

as '**Martensite Reversion Steels**' [65,68,69]. These are ductile **micro- and nanolaminate alloys** that are formed by reheating as-quenched martensite steels (e.g. Fe-Mn, Fe-Ni, Fe-C, maraging or Fe-Cr-C steels) so that segregation-driven reversion from martensite back to austenite occurs at internal interfaces, preferably at the **lath interfaces**, Fig. 11 [145]. The size, elemental partitioning, shape and position of the reversed phases determine the mechanical properties of the bulk compound. These alloys resemble intrinsically formed damask alloys, enabled by a segregation, reversion and partitioning heat treatment. Preceding plastic deformation can profoundly enhance the effect as it provides additional nucleation sites for reversion (see p. 50).

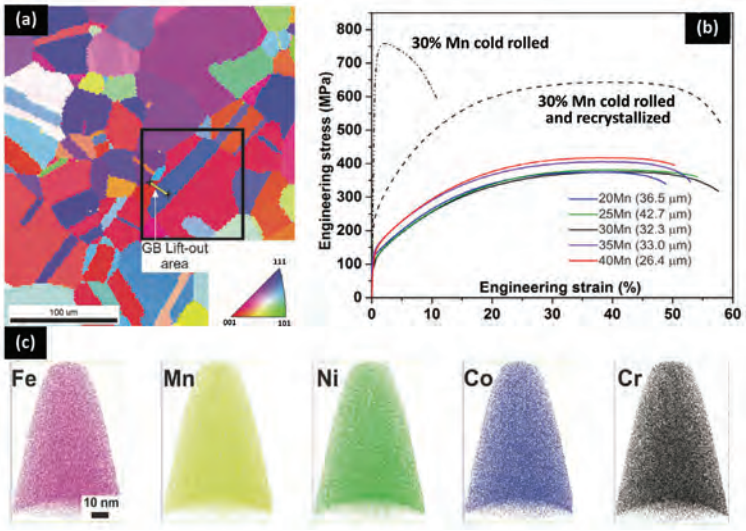

Fig. 10: *Fe_{62}-$Mn_xNi_{30}Co_6Cr_2$ non-equiatomic high entropy alloys (x: variation in Mn) (a) Inverse pole figure map showing the APT lift out region. (b) Stress-strain curves of all alloys: the 30 at.% Mn alloy is shown in cold rolled (64%) and recrystallized (900°C, 10 min) states. (c) APT reveals the materials' compositional homogeneity [95,139-144].*

Similar phenomena occur in **Ti-Mo and Ti-Fe alloys** where β-phase films form between the α-lath portions by a reversion heat treatment, Fig. 12 [132]. The phase transformation and reversion kinetics between the hexagonal α-phase and the bcc β-phase enable the design of laminate microstructures leading to excellent mechanical properties. We studied the effects of different types of reversion treatments in a **binary Ti-4Mo (wt%) model alloy**. We observed a broad variety of microstructure formation mechanisms including diffusion driven allotropic phase transformations as well as shear and/or diffusion dominated modes of martensitic transformations, leading to a wealth of microstructure design options in a simple binary Ti alloy (see p. 50).

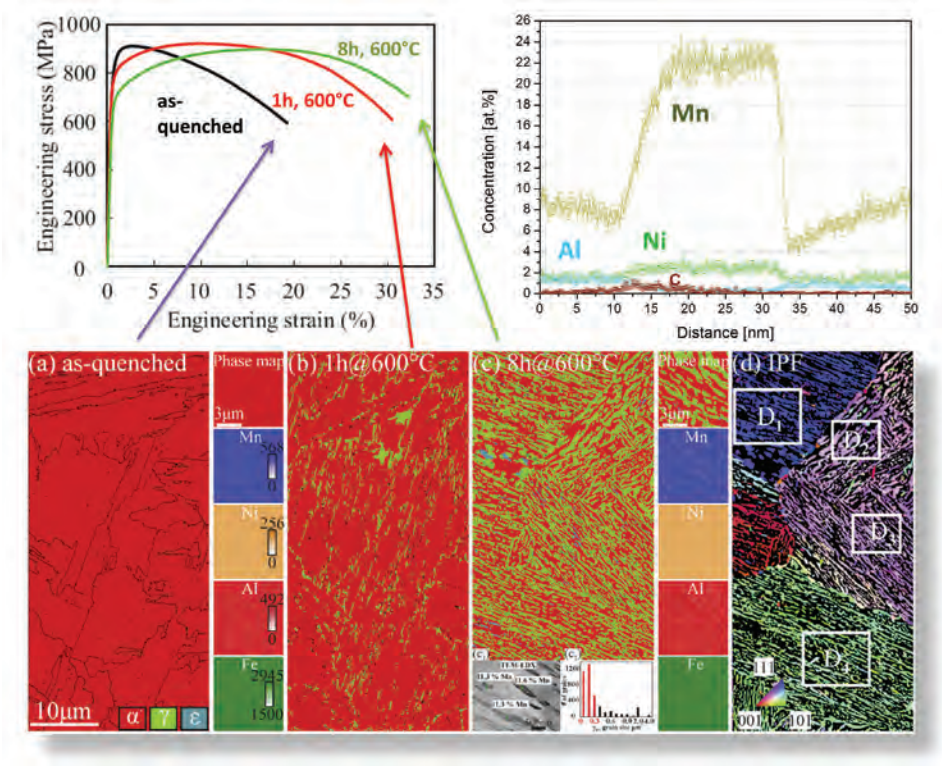

Fig. 11: *Grain boundary segregation followed by confined reversion transformation (revealed by APT) from the as-quenched martensite into austenite enables the design of damask-type martensite-austenite nanolaminate steels where the solute decorated lath interfaces transform back to austenite [145].*

Multilayer nanolaminates

Multilayer nanolaminates are capable of **reconciling strength and ductility** and/or providing toughness or hardness to **substrate surfaces**. We study the nanostructure evolution of metallic crystal-glass [3,8,20] and multi-nitride laminates [89,146] with respect to their mechanical, thermal and compositional stability when exposed to **thermal and mechanical loading**. As

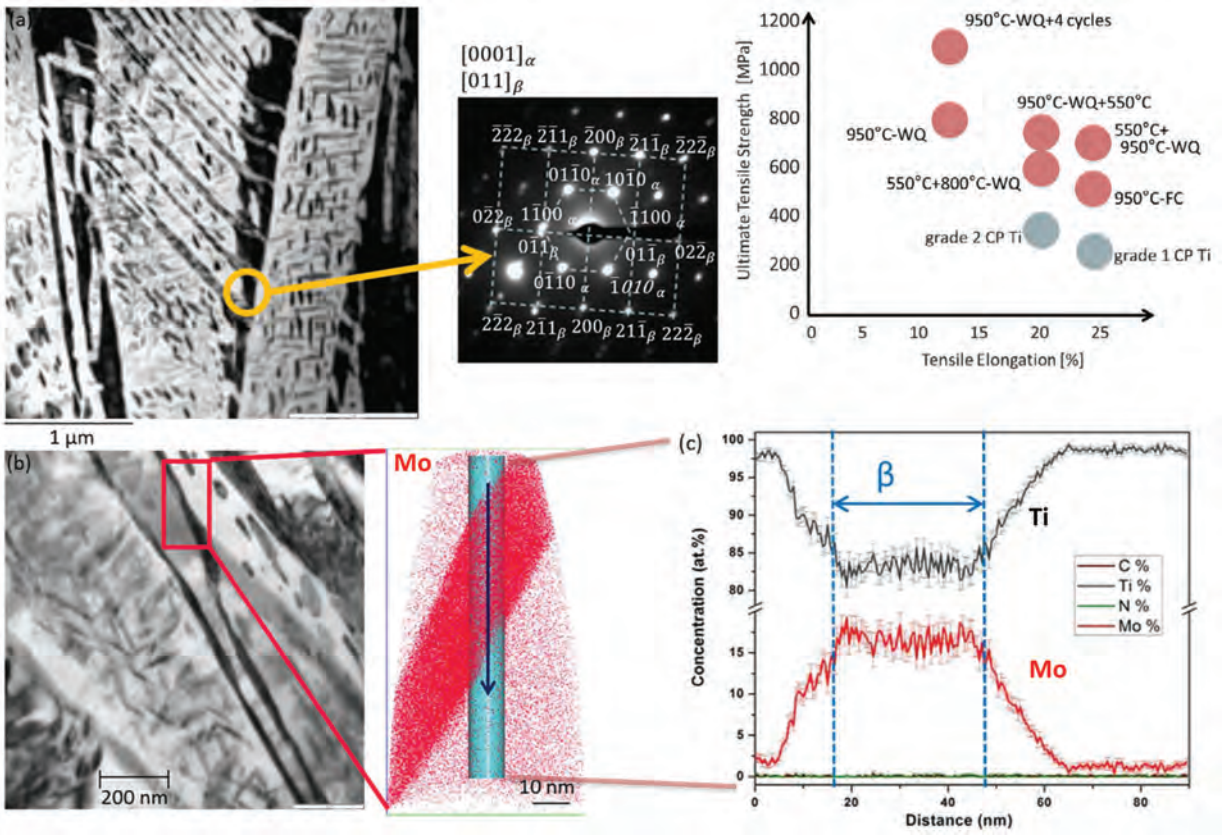

Fig. 12: *(a) Bright-field TEM micrograph and selected area diffraction pattern depicting the near-Burgers orientation relationship observed between the α (hcp) and β (bcc) phases in Ti-4Mo after heat treatment 950°C-WQ + 550°C. (b) TEM bright field image, APT elemental map showing Mo atoms and (c) the corresponding 1-D concentration profile (bin width 0.5 nm) across the Mo enriched layer (cylindrical region of interest in (b)) showing very pronounced partitioning of Mo (red) of about 20 at% into a 20 nm thick b lamellar zone, enhancing its stability against phase transformation. Upper right image: Tensile mechanical properties of Ti-4wt.%Mo after different heat treatments; (CP: commercial purity standard)* [132].

one model system we chose **crystalline-amorphous** Cu–CuZr **nanolaminates** [3,8,20]. We conducted indentation experiments on 10 nm nanocrystalline Cu–100 nm amorphous CuZr multilayers, Fig. 13. By **correlative APT-TEM** we found that crystallographic slip bands in the Cu layers coincide with non-crystallographic shear bands in the amorphous CuZr layers. Dislocations from the crystalline layers drag Cu atoms across the interface into the CuZr layers. Also, crystalline Cu blocks were sheared into the CuZr layers.

In another project, conducted together with J. Neugebauer, we performed **joint APT structural data analysis and quantum-mechanical calculations** in a theory-guided design approach to identify **nanolaminate superlattices** with **extreme-stiffness**, Fig 14 [147]. These superlattices can contain metastable phases which are stabilized by epitaxial constraints. The study combines theoretical and experimental methods to optimize the elastic properties of AlN/CrN superlattices with 4 nm bilayer period. CrN stabilizes AlN in a metastable B1 (rock salt) cubic phase only in the form of a layer that is very thin, up to a few nm. The *ab initio* predicted Young's modulus (428 GPa) along [001] is in excellent agree-ment with corresponding values from nano-indentation (408±32 GPa) (see p. 50).

Micromechanics of high-mechanical contrast materials

Multiphase microstructures containing phases with **high mechanical contrast** are essential in alloy design [35,36,55,56]. Particularly **dual-phase (DP) steels** take a prominent position among high-strength steels, but they are prone to failure. In a series of studies we explored (a) the microstructure evolution during processing, (b) conducted detailed experimental characterization of the micromechanical behaviour and phase co-deformation, and (c) simulated the micromechanical and coarse grained material behaviour. Fig. 15 shows some of the main resulting trends to guide future DP design efforts [40] (see p. 50).

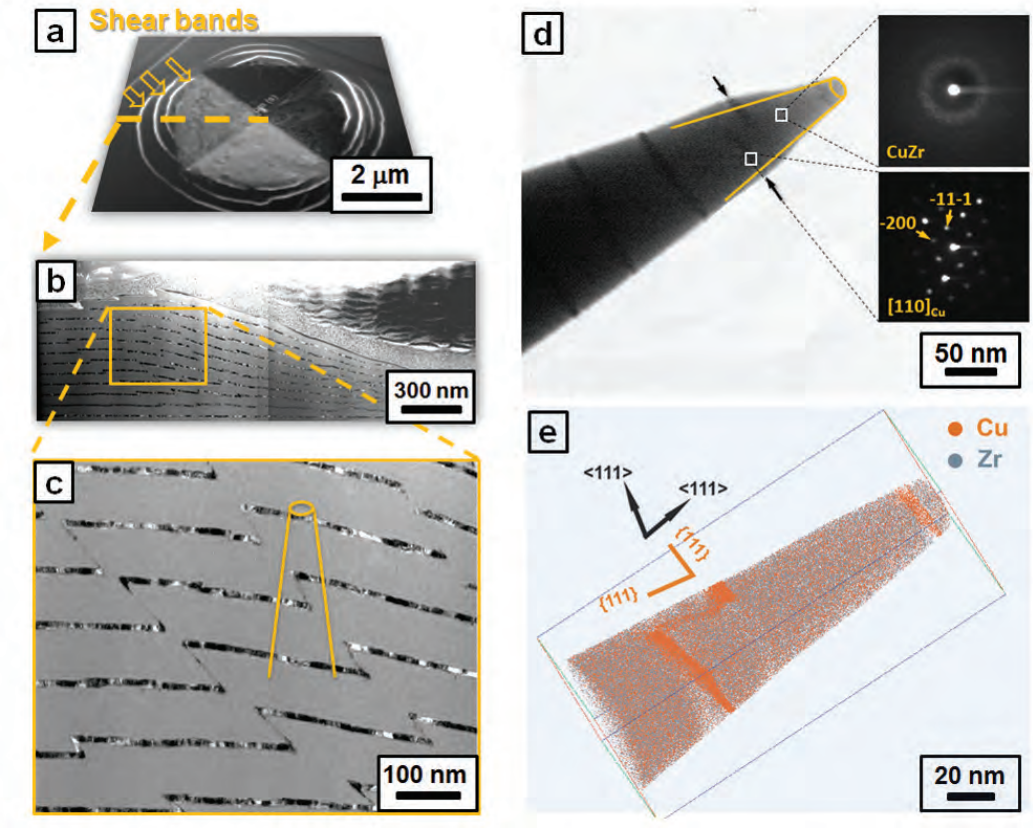

Fig. 13: *(a) SEM view of indented CuZr/Cu nanolaminates. (b) Shear bands. (c) Bright field TEM image of shear bands. Yellow lines mark a region studied by APT. (d) Bright field TEM of an APT tip with CuZr and Cu nanobeam diffraction. Arrows show the shear band region. (e) APT reconstructed volume from the exact APT tip shown in (d)* [3,8,20].

Main Recent Breakthroughs

In several cases we achieved breakthroughs during the past years. While some resulted from **unexpected discoveries** [1], others were harvested from **long term and systematic developments** [24,26,42].

Regarding method development we have established a versatile experimental protocol for conducting site-specific sample extraction in conjunction with **correlated TEM-APT characterization** [1-5,18]. This approach enables profound insights into the interrelationships between structure and composition in complex microstructures at near atomic scale. Examples where this approach enabled basic new insights are the discovery of **linear complexions** [1], atomic-scale analysis of **segregation** phenomena in 5D crystallographic space [5], the observation of para-equilibrium partitioning in **quench-partitioning** steels [128] and interface phase formation in **high entropy alloys** [139].

Similar progress was enabled by rendering the **Electron Chaneling Contrast Imaging** method quantitative by combining it with controlled diffraction conditions (cECCI) [25-27]. It allows the direct observation of crystal defects such as dislocations or stacking faults close to the surface of bulk samples. This technique, which has similarities to dark field TEM, is applied in a SEM and allows probing the first 50–100 nm of material below the surface.

Substantial progress was also made in the field of **mapping hydrogen** with high spatial resolution, hence, correlating trapping sites and damage events with local microstructure features.

In the field of **simulation** substantial progress was made in the field of joint polycrystal and multiphysics modeling. The corresponding software package developed during the past 15 years was released to the public domain as **Düsseldorf Advanced MAterials Simulation Kit** (**DAMASK**) and can be downloaded at **http://damask.mpie.de**. It is used by a number of research groups worldwide [42]. Regarding alloy design we have made substantial progress by introducing the concept of **non-equiatomic high entropy alloys** [95,140-144] and the use of **interstitial alloying** in these materials [81].

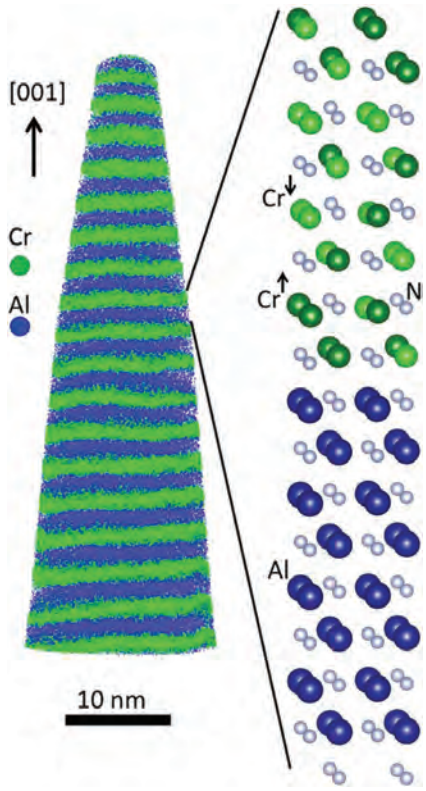

Fig. 14: *Spatial distribution of Cr and Al in an AlN/CrN superlattice measured by APT (left) and the computational model derived from these data (right) for identifying nanolaminate superlattices with extreme-stiffness [147].*

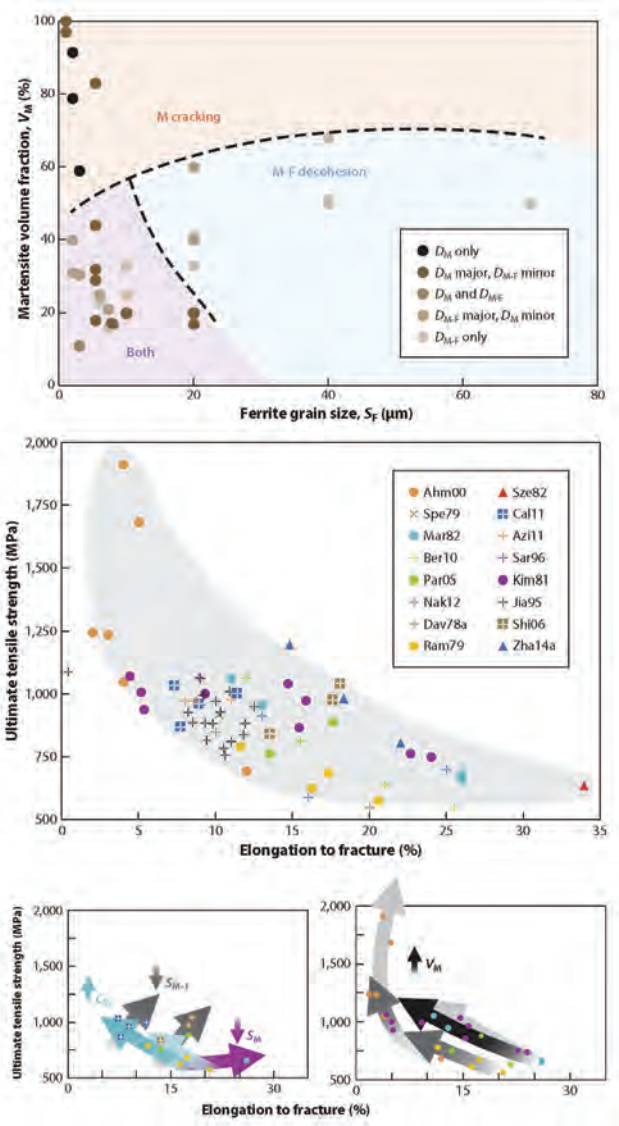

Fig. 15: *Dual-phase (DP) steels: Damage analysis reveals the effects of ferrite grain size (SF) and martensite volume fraction (VM) on the type of damage: martensite cracking (DM) and martensite-ferrite decohesion (DM−F). F and M indicate ferrite and martensite, respectively. Middle row: strength – ductility combinations compiled for a large number of DP steels. The original data and references are provided in [40]. Bottom row: Several trends due to microstructure effects. Abbreviations: CM, martensite carbon content; SM+F, martensite and ferrite grain size; SM, martensite grain size; VM, martensite volume fraction [40].*

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Research Projects in Progress

Ponge, Raabe, Li: OPTIBOS – New developments and optimization of high strength Boron treated steels through the application of advanced Boron monitoring techniques

Cojocaru-Mirédin, Raabe: NanoMatFutur - Optimierung des Wirkungsgrades von Solarzellen basierend auf 3-dimensionalen chemischen Analysen auf atomarer Skala (in collaboration with RWTH Aachen)

Raabe, Fabritius: Generation of multifunctional inorganic materials by molecular bionics "Biogenic ACC Formation: The Mechanism of controlling Phase and Structure of Calcium Carbonate"

Tasan, Grabowski, Raabe, Neugebauer: SMART-MET - Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys

Ponge, Springer, Raabe: Bladestrip - Innovative Werkstoffgeneration für Schneidwaren durch die revolutionäre Fertigungstechnologie Bandgießen

Raabe, Schneider, Dehm, Köhler, Schnabel: Topological Engineering of Ultra-Strong Glasses

Fabritius, Wu: Biomimetic photonic crystals with mechanochromic properties based on cuticular scales of the weevil Entimus imperials

Sandlöbes, Nellessen: Constitutive modelling and microstructural validation for crystal plasticity finite element computation of cyclic plasticity in fatigue (in collaboration with RWTH Aachen)

Zambaldi, Eisenlohr: Characterization and Modeling of the Interplay between grain boundaries and heterogeneous plasticity in titanium

Zaefferer, Raabe: Local texture analysis and crystalline anisotropy in Mn-steels

Sandlöbes, Ponge: Synthesis and Characterization of Fe-Mn reference materials

Choi, Cojocaru-Mirédin, Schwarz, Raabe: Characterization of CIGS Solar Cells by Atom Probe Tomography

Choi, Tytko: Thermal stability of metal nitride superlattices studied by means of Atom Probe Tomography

Sandlöbes, Friak, Raabe, Neugebauer: Fundamentals of the ductilization of Mg alloys microalloyed with rare earth elements

Shantraij, Roters, Eisenlohr, Svendsen, Raabe: Physically based approach for predicting and minimizing damage nucleation in metals

Tarzimoghadam, Ponge: Hydrogen embrittlement in Ni alloys

Wong, Roters: Constitutive modeling of joint TRIP and TWIP deformation of in advanced high strength steels

Zaefferer, Ram: High resolution scanning electron back scatter diffraction experiments and local strain determination in Mn-based steels

Springer, Belde, Baron: Synthesis, alloy design and phase boundary mechanics in multiphase steels

Elhami, Zaefferer: Relationship between microstructure and damage mechanisms in multiphase steels

Tasan, Diehl, Roters: Simulation of the mechanical response of stable dual phase steels

Li, Choi, Goto, Kirchheim, Raabe: Fundamentals of the strength of pearlite

Povstugar, Choi, Tytko, Raabe: Atom probe tomography of the chemical composition of interfaces in Ni-base superalloys

Choi, Tytko, Raabe, Povstugar: Thermal stability of metal nitride superlattices studied by means of atom probe tomography

Varnik, Raabe: Theoretical investigations on shear bands in colloidal glasses

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G. Dehm

Scientific Mission and Concepts

The objective of the newly formed department (October 2012) is to perform basic research on microstructure physics and mechanical properties of structural and functional materials with a focus on small length scales down to atomic dimensions. Our mission is to develop and enhance accurate and quantitative *in situ* nano-/micromechanical test methods with the aim to improve and tailor the mechanical properties of materials by resolving the interplay between microstructure components (e.g. phases, interfaces, dislocations) and the resulting mechanical performance (e.g. strength, ductility, toughness). The materials portfolio which we study comprises alloys, in particular steel and intermetallics, and nanocrystalline materials for structural applications as well as thin films for functional applications (e.g. coatings, flexible electronics, semiconductor devices). The aim of our scientific work is to gain fundamental knowledge on plasticity mechanisms with high spatial resolution, as this provides new insights into deformation phenomena, mechanisms of damage accumulation, and finally crack initiation followed by materials failure, and to use this knowledge to develop design criteria to make materials more robust and reliable. The mechanical techniques we apply range from self-designed micro- and nanomechanical test methods to nanoindentation and nanotribological tests. As a prerequisite, a detailed understanding of the microstructure is required. This is accomplished by applying scale bridging characterization techniques such as X-ray diffraction (XRD) and synchrotron methods as well as scanning electron microscopy (SEM) and advanced scanning/ transmission electron microscopy (S/TEM) methods. Our specialty is to combine both approaches – advanced microstructure characterization and localized mechanical testing – permitting to study the evolution of reversible and irreversible deformation processes “live” during the external stimulus.

The department consists of 5 scientific research groups (see Fig. 1) which closely interact amongst each other and within the institute to contribute to MPIE’s interdisciplinary mission of developing new high-performance materials for use as high-tech structural and functional components. In addition, the research groups also pursue their own scientific agenda to tackle central scientific questions within their research themes. Currently, the department has 4 groups in operation: Dr. Christian Liebscher was attracted from University of California at Berkeley as head of the Advanced Transmission Electron Microscopy group (since April 2015, see p. 27), Dr. Steffen Brinckmann from the Ruhr-Universität Bochum as head of the Nanotribology group (since December 2014, see p. 22), and Dr. Christoph Kirchlechner form the Montanuniversität Leoben (Austria) leads since March 2013 the group Nano-/ Micromechanics of Materials (see p. 26), which

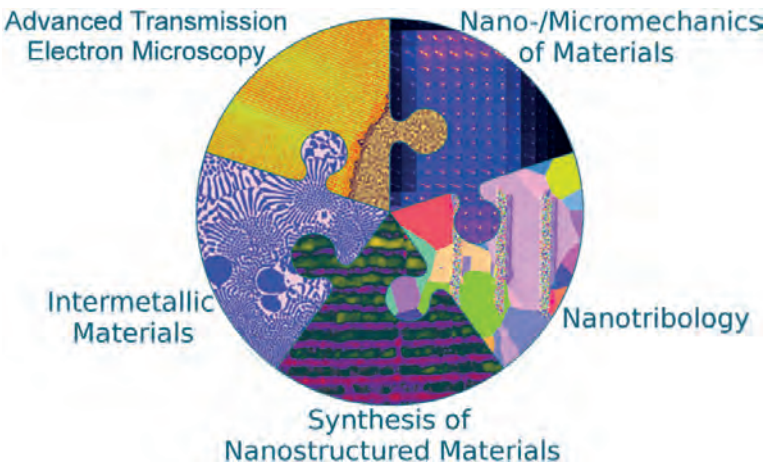

Fig. 1: *Interacting groups of the SN department.*

also includes the XRD and synchrotron activities of the department. The research group Intermetallic Materials was until September 2012 temporarily allocated to the MA-Department (Microstructure Physics and Alloy Design) and transferred with October 2012 into the newly formed SN-Department and is co-headed by Dr. Martin Palm and Dr. Frank Stein. The 5th research group, which will deal with the Synthesis of Nanostructured Materials, will be advanced when the reconstruction work of hall 8/9 and the installation of the new facilities have been finished.

Since its foundation in fall 2012 the SN-Department consequently focused on installing and operating the newly required experimental infrastructure and expedited the necessary reconstruction of hall 8/9 to host the institutes advanced S/TEM facility and a laboratory for TEM sample preparation. The new equipment includes a focused ion beam work station (FIB), a commercial *in situ* mechanical testing platform installed inside the SEM, a self-made nano-/ micromechanical test rig, which is mainly dedicated for µLaue synchrotron diffraction experiments, a nanoindenter system with lateral force sensor for quantitative nanotribological measurements combined with a home-build electrochemical cell. The latter system will allow in future studying the mechanical and tribological behaviour of materials under environmental conditions - synergistically with the GO-Department (Interface Chemistry and Surface Engineering). “Live” observation of microstructural changes caused by external stimulus can be probed with dedicated TEM holders (liquid cell, indentation, and a heating holder) opening a window into the nanometer length scale of materials phenomena in corrosion science, mechanical properties, and thermodynamics. Last but not least, an aberration corrected S/TEM for structural and analytical microstructure characterization at the atomic level went into scientific operation in July 2015. The new advanced S/TEM equipment complements MPIE’s advanced characterization infrastructure, especially the 3-dimensional atom probe tomography (APT) facilities (MA-Department) with its unprecedented chemical sensitivity, by permitting atomic resolved structure and bonding analyses of phases, interfaces and other microstructural components of high performance materials.

Although the start of a number of new facilities within a short period of time is a challenge by itself, several major scientific achievements have been accomplished by our research in the last 3 years. In the field of Nano-/ Micromechanics of Materials we have made significant progress in performing accurate miniaturized fracture mechanics tests. The lack of standards necessitates determining the accuracy and limits of the applied testing techniques. We used silicon as a well-known reference material to benchmark 4 different miniaturized fracture testing schemes [1]. Based on the findings we were able to expand the methodology to metallic glasses in form of thin films to uncover the origin of brittleness and ductility of such materials [2] within an interdisciplinary cooperation including the MA-Department and the RWTH Aachen with the recently founded Max Planck Fellow Group Self Reporting Materials headed by Professor Jochen Schneider.

Our advanced synchrotron experiments on heavily wire drawn pearlitic steel uncovered an unexpected phase transformation from ferrite to martensite as a consequence of the decomposition process of the cementite phase. Dr. Soundes Djaziri and Dr. Christoph Kirchlechner discovered by an in-depth analysis of the diffraction data concerning texture, internal strain, and lattice parameters of pearlitic wires, that for wires exposed to drawing strains exceeding 200% the ferrite lattice becomes tetragonally distorted. The close collaboration with the departments MA and CM (Computational Materials Design) led to a profound understanding of the origin of the transformation and to the conclusion that the tetragonal ferrite indeed corresponds to a strain induced martensite. APT measurements revealed that the carbon content inside the ferrite grains exceeded the solubility limit, which at a certain concentration level leads to a spontaneous carbon ordering at specific octahedral sites of the bcc lattice, as found out by computational modelling performed by the CM-Department. This corresponds to the carbon ordering in martensite created by quenching austenite. Thus, the decomposition of cementite in the pearlite wires causes a carbon supersaturation of ferrite, which in turn leads to the strain-induced martensite formation – a new mechanisms which was previously overlooked.

The interplay between microstructure physics and mechanical properties is also at the core of our studies on interface plasticity and fracture [3-13]. As an example, dislocation transmission across twin boundaries was revisited by *in situ* and *post mortem* µLaue diffraction, SEM and S/TEM imaging – always combined with quantitative global stress and strain measurements. All our experiments revealed that the coherent Σ3(111) Cu twin boundary exerted no measurable increase in strength compared to single crystals of the same size and orientation, a result opposing molecular dynamic predictions in the literature which claim that shear stresses of more than 400 MPa are required for dislocation transmission.

Grain boundaries intersected by scratches permit in nanotribology to study dislocation transmission, absorption, nucleation or pile-ups at interfaces by analyzing the slip markings on the surface and changes in grain orientation by electron backscatter

Fig. 2: *Members of the SN department (picture taken in Sep. 2015).*

diffraction (EBSD) in the SEM [14,15]. Also in thin film systems like metal films on polymers the interface is detrimental for the film adhesion and mechanics. We studied the influence of Cr adhesion layers for Cu films on polyimide substrates and found out that although the Cr layer promotes adhesion it significantly deteriorates the resistance of the Cu against failure by cracking. Channel cracks forming in the brittle adhesion layer lead to significant stress concentrations in the adjacent Cu film causing failure at much lower strains than for Cu films directly applied to the polyimide substrate [16,17]. This finding has significant influences for flexible electronic devices.

The new department is already well connected within MPIE and has also established contacts to the Ruhr Universität Bochum (RUB), where G. Dehm is associated at the Materials Research Department and the Institute for Materials (Institut für Werkstoffe) as a professor (Außerplanmäßiger Professor). The SN-Department hosts the research group High Temperature Materials headed by Prof. Gunther Eggeler, which continues the previously established Max Planck Fellow Group that expired in the beginning of 2015 after completion of its 5-year funding period. Interactions with Prof. Alfred Ludwig (RUB) within the International Max Planck Research School for Surface and Interface Engineering in Advanced Materials (IMPRS-SurMat) on combinatorial thin film Cu alloy design for energy systems, Prof. Jochen Schneider (RWTH Aachen) on hard coatings and metallic glasses, as well as Prof. Mick Feuerbacher (Jülich) and Prof. Easo George (RUB) on high entropy alloys have been realized. The department also started to interact with steel companies and was host for two 1 year secondments of industry researchers on Precipitate characterization in electrical steels and on Nanomechanics of steel. In addition, we are active in acquiring third party funds such as the EPPL-project (Enhanced Power Pilot Line) funded within the ENIAC Joint Undertaking to strengthen Europe's leading position in power semiconductors, DFG projects on µLaue investigations of dislocation-grain boundary interactions (Dr. C. Kirchlechner) and on novel Fe-Al alloys with fine-scaled lamellar microstructures (Dr. F. Stein), and a collaboration with 5 European industrial partners (HERCULES-2) within the framework of Horizon 2020 on Intermetallics for engine applications (Dr. M. Palm).

The SN-Department holds regularly seminars where the students, postdocs and senior scientists report on their current research topics, and once a year a department retreat jointly with the independent research group Nanoanalytics and Interfaces (Prof. Christina Scheu) and external scientists is performed to discuss the individual research topics and to strengthen interactions within the department. Joint interdepartmental seminars on topics of

relevance for more than one department provide the major platform for in-house collaborations on specific strategic topics. Additionally, workshops and conferences are organized by SN-Department members to foster international collaborations and exchanges. Examples are the Mecano General Meeting „Mechanics of Nano-Objects“ (18 - 19 July 2013) at MPIE organized by G. Dehm, the workshop on “Bridging the scales in tribology and wear” jointly organized by S. Brinckmann and M. Valtiner (GO-Department), the conference “Intermetallics” 2013 and 2015 (30 September - 4 October 2013 and 28 September - 02 October 2015, Kloster Banz) co-organized by F. Stein and M. Palm, the Symposium “Structure and dynamics V: Mechanical properties at small scales” at Condensed Matter CMD25-JMC14 (24 - 29 August, Paris, France) co-organized by G. Dehm, the “Intermetallics“ Technical Committee Meetings of the German Society for Metals (DGM) at the Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, 10 Jan. 2013, and at MPIE, Düsseldorf, 26 Feb. 2014, both organized and chaired by M. Palm, who also was head of this committee until 2014, and the workshop on “Rasterkraftmikroskopie und nanomechanische Methoden” co-organized by C. Kirchlechner (held at MPIE 27 - 28 Feb. 2014 and in Darmstadt on 5 - 6 Mar. 2015), who became recently head of this technical committee of the DGM.

The success of the scientific work of the members of the SN-Department is reflected by numerous invitations to lectures at conferences and university/institute colloquia. Prestigious examples include two invited talks from C. Kirchlechner and G. Dehm at the Gordon Research Conference on Thin Film & Small Scale Mechanical Behavior (2014), an invited talk by C. Kirchlechner at the ECI conference Nanomechanical Testing in Materials Research and Development V (2015), and invited talks at Fall MRS meetings (2013, 2014, 2015) by C. Kirchlechner and G. Dehm. In 2015, B.N. Jaya presented invited talks at the International Conference on Metallurgical Coatings and Thin Films (ICMCTF 2015) and the 17th International Conference on the Strength of Materials (ICSMA 17), and G. Dehm gave an invited talk at the Frontier of Electron Microscopy in Materials Science (FEMMS 2015) and a keynote lecture at EUROMAT 2015.

We also promote career opportunities for the young scientists in industry and launched a new series at MPIE jointly with the MPIE PhD representatives called Career Talks. The first career talk took place on 27th of March with the ThyssenKrupp Steel Europe AG explaining their job portfolio followed by a get-together, where in an informal atmosphere contacts were exchanged. This was followed by an onsite visit at ThyssenKrupp Steel Europe AG in Dortmund on 4th of May 2015. Due to the positive response of all involved parties, 2-3 career talks per year with further industrial partners are planned. The next ones are with McKinsey and Company in October 2015 and with BASF in November 2015 (see p. 58).

In the following, the research activities of the research groups of the SN-Department are provided and selected projects summarized.

Scientific Groups

Nano- and Micromechanics of Materials (C. Kirchlechner)

The Nano- and Micromechanics Group - More than a mechanical microscope. Advances in micro sample preparation, micromechanical testing and nondestructive microstructural characterization enable us today to explore the mechanical behaviour at hitherto unreached small dimensions. Aim of our research is to study the mechanical behaviour of materials at the microstructural length scale. Our work is stimulated by various questions in advanced material science, such as (i) the origin of size-dependent mechanical behaviour of single crystals, (ii) the quantitative understanding of individual deformation mechanisms governing plasticity in complex microstructures, (iii) the quantification of damage accumulation in individual microstructural constituents during cyclic loading and, finally, (iv) the micro fracture behaviour of phases and interfaces.

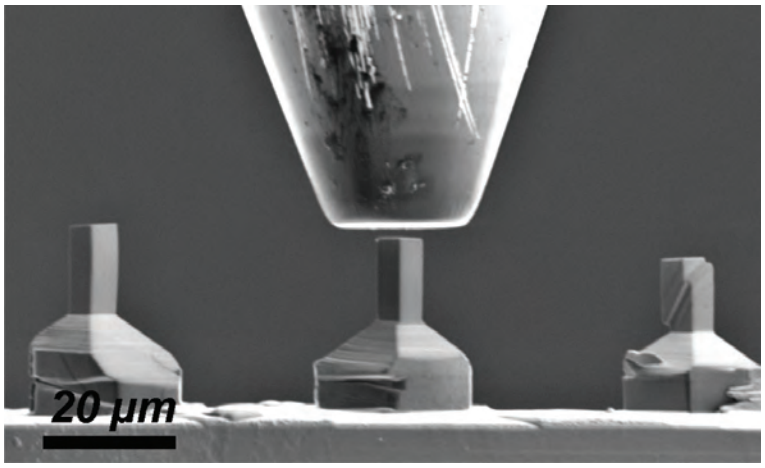

Fig. 3: *SEM images of single and bi-crystalline copper micropillars. The two outer pillars are single crystalline references, the centered one being ready for loading by the indenter is bi-crystalline.*

The intended purpose surpasses measuring local mechanical properties by far. A central aspect of our work is to interlink the underlying and evolving defect structures (e.g. dislocation types and densities, length and density of cracks and crack networks, etc.) with the mechanical response. This requires advanced characterization methods and dedicated *in situ* equipment, which are both developed in house.

Buildup of micromechanical capabilities. After the group was found in spring 2013, the main focus was put on the buildup of *in situ* micromechanical capabilities (see p. 30). Micro loading rigs for *in situ* SEM and *in situ* µLaue diffraction (SSD2) performed at the European Synchrotron Radiation Facility (ESRF), as well as a focus ion beam system (Zeiss Auriga®, Zeiss Oberkochen) were successfully implemented in 2013. Characteristic sample dimensions of these machines are ranging from hundreds of nanometer to tens of micrometers. The aforementioned methods permit deep insights into the cumulative behaviour of dislocations during mechanical loading and therefore are of central importance for our group. Complementary, mid 2014 we successfully implemented a Hysitron PI-95 PicoIndenter® being able to perform *in situ* TEM, which gives us a detailed view on individual dislocations and their interaction with other lattice defects. Our today's equipment is well able to measure important microstructural parameters during *in situ* deformation. Examples are monitoring sample shape changes (*in situ* SEM), deviatoric strains and strain gradients as well as the cumulative behaviour of geometrically necessary dislocations (*in situ* µLaue) and the interaction of individual dislocations with other defects (*in situ* TEM). The complementary characterization methods span over the most important hierarchical levels in structural materials, which is prerequisite to formulate mechanisms-based material laws.

Size-dependent crystal plasticity. The size dependence of single crystals had been investigated during the last decade. Even though not formulated as a mechanism based material model, the importance of dislocation source sizes and source availability is well known and suggested by several studies. Remaining questions in this field are the impact of elevated temperatures on the size dependent behaviour, as well as the size scaling of non-cubic crystal structures. As one research highlight we aim for understanding of the size dependent material properties in tetragonal body centered tin. Particularly interesting in this material – being in our focus due to the demand of lead free solder joints of the automotive electronic industries – is that the operating slip systems are yet unknown, and that our experiments can be conducted at very high homologous temperatures of 0.6. The main results are (i) that hardly any dislocations are stored during deformation, (ii) that the size scaling exponent is close to a theoretical value of -1 and finally, (iii) that slip is highly anisotropic with different slip systems being operated in different crystallographic loading directions [18].

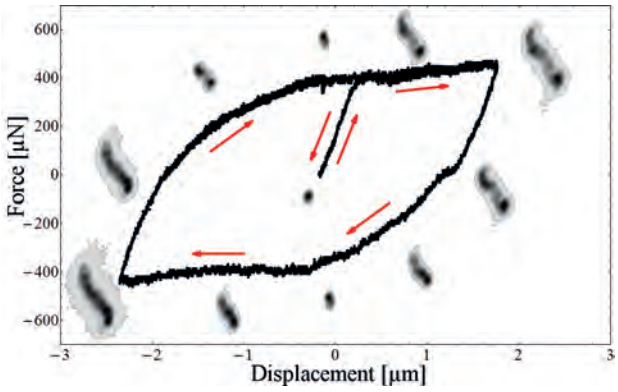

Fig. 4: *Cyclic force displacement curve of a micron-sized, single crystalline bending cantilever with superimposed Laue images. Initially, the Laue spot is circular documenting the lack of geometrically necessary dislocations (GNDs). During beam deflection, GNDs are stored and are forming subgrains within the probed volume. Interestingly, backbending leads to significant reduction of the stored GNDs with negligible GND content in straight beams [19].*

Grain-boundary dislocation interaction mechanisms. Another research highlight and one of the main objectives of the group is to understand grain-boundary (GB) dislocation interaction mechanisms. For this purpose, bi-crystals with specific grain-boundaries are grown by a Bridgman furnace or extracted from well-recrystallized polycrystals. Currently we focus on Cu as a model material. Miniaturized compression (see Fig. 3) and tensile samples with sizes ranging from 500 nm up to 15 µm are produced by FIB milling. During *in situ* testing the piling up of dislocations at the GB, their annihilation at the GB as well as the slip transfer of dislocations through the GB into the next grain are quantified. It is our aim to understand the GB-dislocation interaction in a broad context: various grain boundary types, e.g. coherent Σ3 (111) twins, general large angle grain-boundaries allowing for slip transfer or being strong obstacle for dislocation transfer, and small angle tilt grain-boundaries are tested. In case of the coherent Σ3 (111) twin loaded in <110> we observed dove-tail shaped slip lines where dislocations cross-slipped from one into the second grain. Surprisingly, the slip transfer mechanism does not have any impact on the mechanical behaviour of the twin boundary compared to the single crystalline references [4]. Furthermore, no pronounced pile-up was observed during *in situ* TEM [7] and µLaue diffraction experiments, which suggests that the cross-slip of dislocations through the twin-boundary is not strength dominating at this size regime.

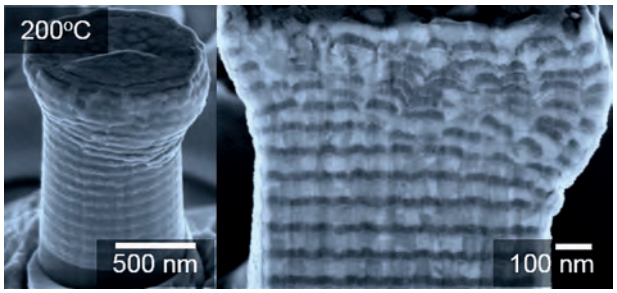

Fig. 5: *Nano-laminated pillar with 66 nm Cu // 33 nm Cr after deforming it to roughly 20% engineering strain (left: full pillar; right: cross-section) [21].*

Besides monotonic loading, structural components have to withstand cyclic loading during service. During the past years we have implemented micro-fatigue experiments on single crystalline micro-bending beams [19] and polycrystalline microsamples [20] to study the impact of cyclic strain gradients as well as the role of a limited number of grain-boundaries on the cyclic behaviour of materials. In the single crystalline bending beams, an almost full reversibility of dislocation multiplication and annihilation can be observed for special sample orientations. This can be seen by the fully reversible peak broadening presented in Fig. 4. However, the reversibility is strongly dependent on the character of dislocation pile-ups. Thus, the geometric orientation of interfaces with respect to the slip systems defines if fatigue damage accumulates or not.

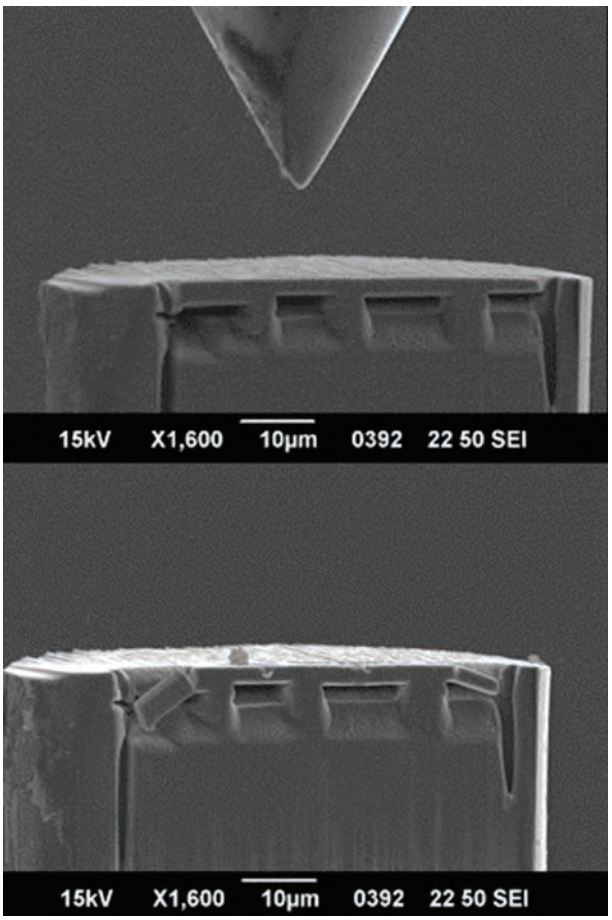

Fig. 6: *Micro-fracture cantilevers milled into a drawn pearlitic steel wire before (top) and after (bottom) fracture experiments.*

Small-scale mechanical behaviour of complex microstructures. Superior performance with multiple different loading and application scenarios (e.g. simultaneous exposure to load and temperature, load and radiation, or current and heat) require complex microstructures. Nano-laminated thin films are a promising candidate, but thorough phenomenon based knowledge is still lacking. To gain deeper insight Cu-Cr thin films with individual layer thicknesses less than 100 nm had been deposited by molecular beam epitaxy. The systems had been analyzed by advanced TEM techniques (SN-Department, Advanced Transmission Electron Microscopy group) and deformed at temperatures up to 300 °C, whereas the high temperature experiments had been performed in collaboration with the EMPA (Swiss Federal Laboratories for Materials Science and Technology) in Thun, Switzerland. An example of a deformed micro specimen is presented in Fig. 5. One of our findings was that the strength surpasses values as predicted by the confined layer slip model or Hall-Petch strengthening [21].

Fracture mechanics at the micron scale. Down-scaling standard fracture mechanical experiments to the micron scale is not straight forward: The size of the plastic zone with respect to the sample size, the impact of friction and the ability to perform geometrically well-defined loading experiments had been questioned ever-since the first micro-fracture mechanical experiments had been shown. This problem gets more and more relevant since various different loading geometries had been proposed. Consequently, the first step within the Nano-/ Micromechanics of Materials group was to compare results of available micro-fracture geometries to the known fracture toughness of bulk silicon [1]. Main and surprising outcome of this study is, that – if the plastic zone size is of negligible size and the experiment is performed in a geometrically well-defined way – all tested geometries yield comparable and within the experimental scatter accurate fracture toughness values (between 0.75 and 0.89 $MPam^{1/2}$). But still, milling time, sensitivity to misalignments and experimental errors, as well as the machine performance important for stable crack growth favors one over the other approach.

Since that proof of principals several projects within the MPIE and with international collaborators had been started to explore the fracture toughness of metallic glasses (MA-Department and RWTH Aachen, Germany, see p. 143), of Si and SiO_2 at non-ambient temperatures (EMPA, Thun, Switzerland)

and of multilayered hard-coatings (TU Wien, Austria). Also the fracture toughness of drawn pearlitic steels wires, as shown in Fig. 6 had been explored. At low drawing strains (<3) the assumption under linear elastic fracture mechanics are invalid and we are currently not able to provide J_{IC} measurements in these systems. However, drawing makes the wire increasingly brittle plateauing at roughly 10 MPam$^{1/2}$. Interestingly, the drop in fracture toughness goes hand in hand with an observed tetragonalization of the ferritic iron and a supersaturation of carbon (MA-Department), which had been proofed by our dedicated monochromatic synchrotron experiments and atomistic simulations (CM-Department) [22].

Adhesion properties of metallic thin films on compliant substrates. Besides studying the mechanical response of FIB-milled samples, also approaches to study plasticity and fracture of thin films had been conducted. Examples are the role of an adhesion promoting chromium interlayer on the mechanical performance of a copper layer [17]. Therefore, three film thicknesses (50,100 and 200 nm) were deposited with and without a 10 nm chromium layer on polyimide. Synchrotron-based powder diffraction applying the sin²ψ method was used to measure the (copper) film stresses in longitudinal as well as transversal direction during tensile testing. At low strains all films follow the smaller-is-stronger trend, thus being well within our expectations. However, in the film systems with adhesion promoting chromium layer the film stresses rapidly drop at low strains. In all cases this was caused by the mechanical failure of the brittle chromium interlayer. In the thinner copper films (50 nm and 100 nm thick) the copper was not able to prevent through channel cracks as presented in Fig. 7 leading to a total electrical failure of the film systems. In contrast, the 200 nm film was able to stop crack propagation to a certain extend and thus, its behaviour does not significantly differ from the films without adhesion promoting interlayer. Our experimental findings had been supported by cohesive zone modelling performed by the groups of Prof. Rammerstorfer (TU Wien, Austria) and Prof. Fischer (Montanuniversität Leoben, Austria). Similar experiments are currently under way to explore the ability of phase transformations in a cobalt based system to act as failure preventing mechanism.

Outlook. In the future, our now well established setup will be applied for several advanced questions in materials science across the SN-Department and other research groups from the MPIE. Examples are (i) a continuation of investigating the dislocation grain boundary interaction mechanisms and its impact on fatigue at the micron scale (ii) the mechanical behaviour of multilayered film systems with designed interfaces (iii) the ability of phase transformations to enhance fracture properties at the micron scale and (iv) finally, implementing high temperature capabilities.

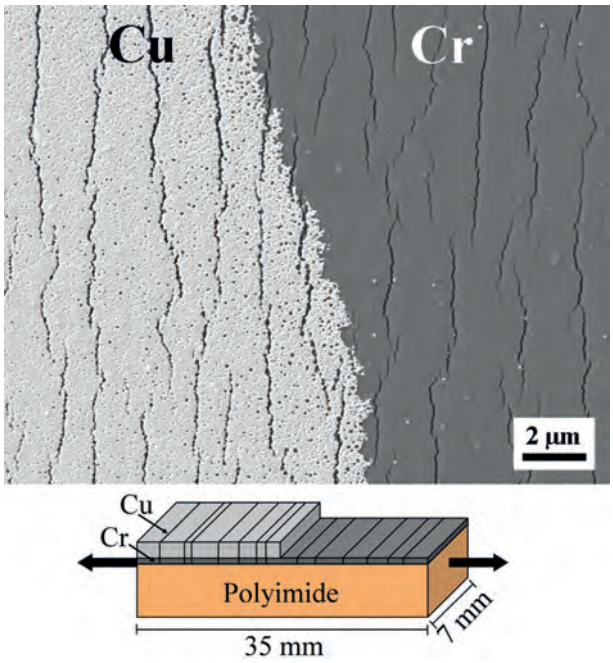

Fig. 7: *Crack network in a thin film system consisting of a polyimide substrate with 10 nm chromium interlayer and 50 nm copper layer as published in [17].*

Advanced Transmission Electron Microscopy (C. Liebscher)

Introduction and mission.

The research of the newly established group Advanced Transmission Electron Microscopy revolves around the application and development of advanced TEM techniques to investigate structural and functional materials from the atomic level up to mesoscopic length scale. We are specifically interested in understanding the atomistic and chemical structure of solid-state defects and interfaces in materials and their behaviour and interaction observed under *in situ* conditions. This fundamental knowledge serves as a solid comparison for atomistic predictions (e.g. by the CM-Department) and is used to develop materials design strategies tailoring desired properties by manipulating materials on the atomic scale. Advanced TEM offers the essential techniques to investigate and manipulate materials on this length-scale bridging approach. Aberration-corrected electron microscopy enables the structural characterization of materials with atomic resolution containing all necessary information about crystallography, chemistry and electronic structure of defects, interfacial phenomena and precipitate structures. In combination with *in situ* techniques the structure and properties are sampled simultaneously closing the missing link between microstructure and properties.

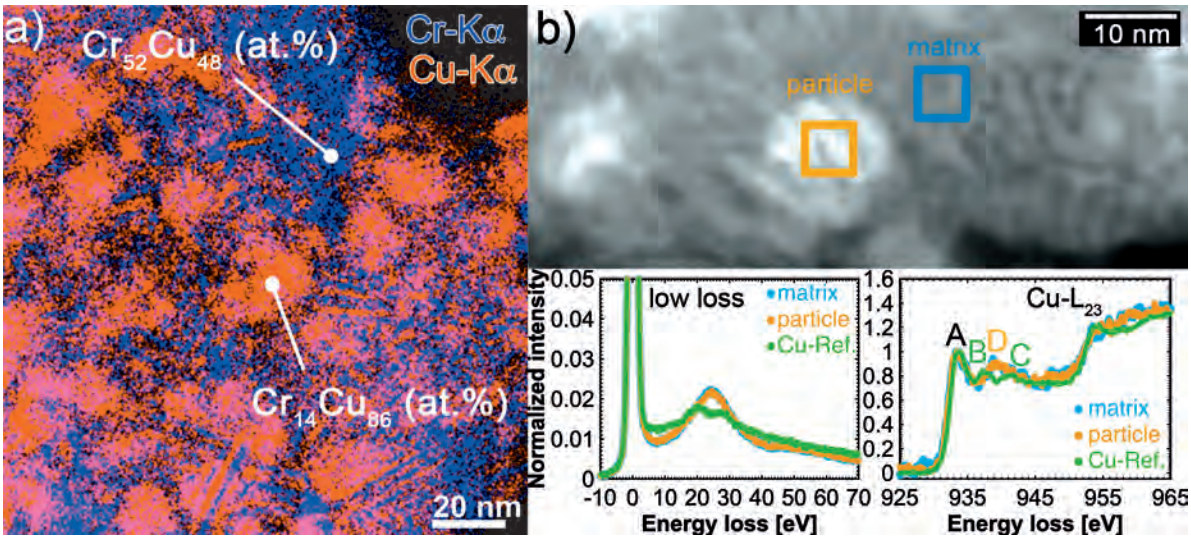

Fig. 8: *a) STEM-EDS elemental maps of an as-deposited $Cu_{66}Cr_{34}$ sample. The microstructure is decomposed into Cr-rich (matrix) and Cu-rich (particle) regions. b) HAADF-STEM image and corresponding low and core loss spectra acquired with dual channel EELS. The spectra are compared to a pure fcc-Cu reference sample. The Cu-L_{23} edge of fcc-Cu shows 2 distinct peaks B and C after the L_3-edge (A). The near edge fine structure for bcc-type Cu exhibits only one peak D after the L_3-edge due to a difference in bonding characteristics.*

Facilities. The group utilizes three TEMs. A FEI/Phillips CM20 with LaB_6 emitter is used for conventional diffraction contrast imaging and electron diffraction experiments. A JEOL JEM2200FS with Schottky field emitter and in-column omega energy-filter enables the characterization of materials with lattice resolution. In addition, the JEM2200FS is the main platform for *in situ* TEM experiments with three available third party *in situ* solutions:

- in situ heating experiments with nanometer resolution are performed with a MEMS-based (Micro-Electro-Mechanical-Systems) DENSsolutions double-tilt heating holder allowing temperatures up to 1200 ºC.
- The nano-mechanical properties and related deformation behaviour are probed with a Hysitron PI 95 PicoIndenter (force resolution of ~200 nN and displacement resolution of ~1 nm).
- The real-time behaviour of materials in liquid electrochemical environment is studied in a Protochips Poseidon 210 holder in cooperation with the GO-Department (Dr. K. Mayrhofer and Dr. N. Hodnik).

A probe-corrected FEI Titan Themis is commissioned and fully operational since July 2015. Through its C_s-probe corrector, the microscope is mainly dedicated for atomic resolution scanning TEM (STEM) enabling a resolution down to 0.07 nm. The microscope combines a monochromated, high-brightness electron gun with a C_s-probe corrector and high-resolution energy-dispersive X-ray spectroscopy (EDS) detectors and an electron energy-loss spectroscopy (EELS) detector (see p. 32). The TEM facilities are complemented by the arrival of an image-side corrected FEI Titan Themis estimated for mid 2016.

Although the new group leader started at 1st of April 2015, several research projects within the themes of the Advanced TEM group had been started previously and selected examples are described below.

Structure and stability of nanocrystalline alloys. In a current project, we analyze the phase stability and segregation behaviour of super-saturated solid solutions of fcc Cu and bcc Cr. Exceeding the solubility limit and “stabilizing” grain boundaries by segregation is a novel route to obtain nanocrystalline grain sizes and prevent rapid coarsening during thermal exposure. For the system Cu-Cr the mutual equilibrium solubility is below 0.8at%. However, by co-deposition of both elements we managed to obtain single phase bcc thin films consisting of extremely high Cu concentrations (e.g. 66at%Cu34at%Cr) as proofed by electron diffraction and analytical TEM [23]. The electronic structure of the Cu L_{23} edge of the bcc structure reveals differences compared to fcc Cu and is under further investigation by us in cooperation with Dr. C. Freysoldt (CM-Department), as illustrated in Fig. 8. A super-saturated fcc CuCr alloy can be obtained up to 4 at.% Cr and remains fcc at temperatures of 300°C. At temperatures of 400 to 500°C film decomposition takes place via nucleation and growth of Cr precipitates. In addition, the *in situ* TEM experiments permitted to determine the Cr diffusion coefficient and an apparent activation energy of 157±4 kJ mol^{-1} indicating grain boundary diffusion as the predominant diffusion path [24].

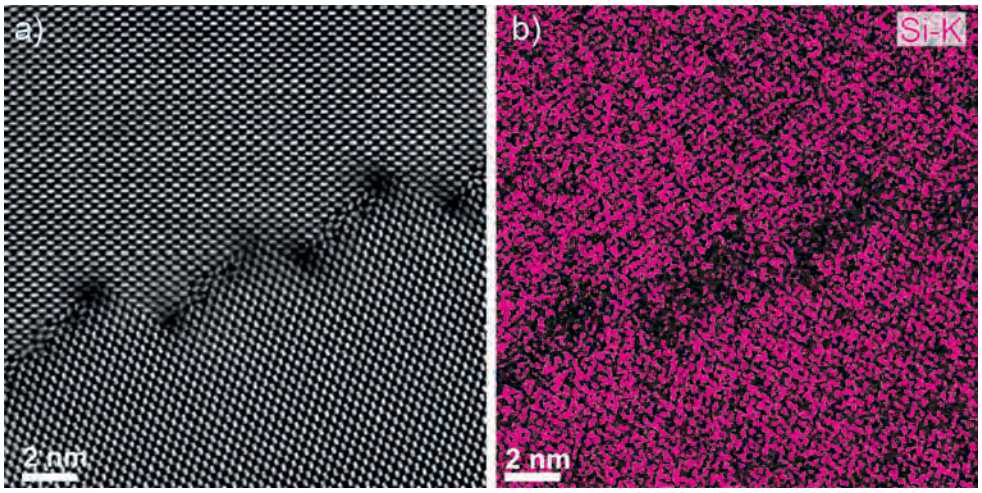

Fig. 9: *a) HAADF-STEM image of a ∑ 3{112} grain boundary extracted from an intentionally doped multicrystalline silicon wafer. Faceting and structural variations along the grain boundary are clearly resolved. b) Lattice fringes from the Si grains are observed in the STEM-EDS elemental map of Si. The Si EDS-signal decreases in certain regions along the grain boundary indicating a lower occupancy of the Si atomic columns. The samples are provided within a collaborative project with A. Stoffers and Dr. O. Cojocaru-Mirédin of the MA-Department.*

Peculiarities of metal-oxide interfaces. Of central interest in our research are interfaces, especially between dissimilar material classes as this is technologically relevant (hard coatings on metals, oxide layers on metals, metallization layers on polymers or insulators), but also scientifically rewarding as interfaces often control the resulting mechanical, tribological and functional properties. In cooperation with the Erich Schmid Institute of Materials Science (Dr. Z. Zhang, Leoben) we recently determined the atomic structure of the interface between Cu (001) and MgO (001) [25]. Cu-MgO serves as a model system for an interface which has to accommodate a large lattice mismatch – in this case more than 14%. The geometric dislocation network forms along <100> directions with Burgers vector ½ a_{Cu} <010>. Cu-O bonds which form in the coherent regions were determined to be 216 ± 8 pm in accordance with density functional calculations performed by Dr. Yao Long (Laboratory of Computational Physics, Bejing) [25]. At the Cu lattice directly adjacent to the MgO modulations of the (002) lattice plane spacing compared to bulk Cu are observed which fade of after 6 to 7 atomic layers. The resolved contraction and expansions are explained by local electronic charge redistribution causing alternating repulsive and attractive forces. In addition, the strain field of the misfit dislocations leads to large rearrangements in the atomic Cu distances adjacent to the dislocation cores with up to 60 pm difference between the shortest and longest Cu-Cu separation distance [25]. Such high precision measurements became only possible with the new generation of TEM instrumentations due to the spherical aberration correction of the imaging system.

Outlook. In the next years, the research of the Advanced TEM group will focus on several themes where high precision structural, chemical, and bonding information is required - embedded in close collaborations within MPIE - to advance the understanding of materials properties. This includes:

- A fundamental investigation of the atomic structure of interfacial phenomena and the impact of segregation, temperature and mechanical load on the interfacial structure.

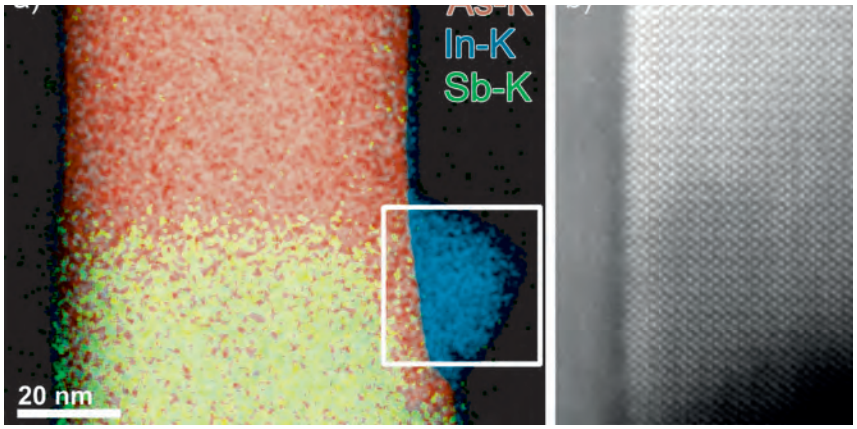

Fig. 10: *a) Interface of a semiconducting InAs-InAsSb nanowire resolved by STEM-EDS. An In-rich droplet is observed to form at the interface between the Sb-rich and Sb-lean regions. b) An atomic resolution HAADF-STEM image of a similar droplet resolving its lattice structure. The project is in cooperation with Dr. P. Krogstrup, University of Copenhagen, Denmark, providing the nanowire samples.*

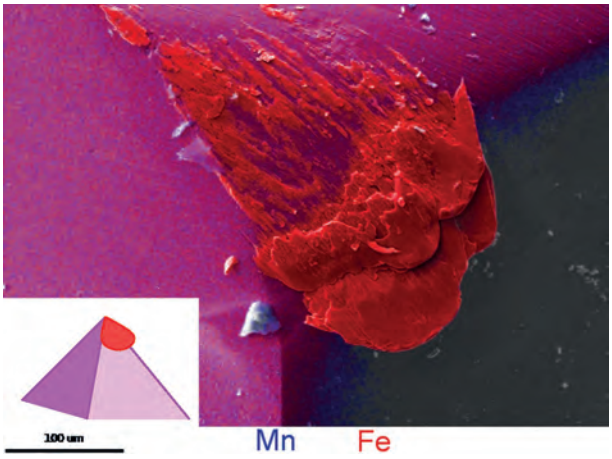

Fig. 11: *Adhesion of Fe on a stainless steel microasperity after scratching. The ferrite is coloured in red, while the stainless steel is a mixture of the blue manganese and red ferrite. The EDS map is overlayed on the SE-SEM image.*

- Coupling of atomic resolution imaging with the development of large-scale image simulations to reveal the three dimensional atomistic structure of complex material systems and to establish a direct connection to theoretical atomistic simulations.
- Resolving the atomic structure of substitutional and interstitial solutes in grain boundaries and their impact on the nano-scale mechanical properties (Fig. 9).
- Basic investigation and understanding of the deformation behaviour of nano-sized micro-structures and defect/interface interactions.
- The effect of alloying behaviour on the atomic and electronic structure in metastable phases, the corresponding microstructural stability and related mechanical properties.
- The design and generation of interface domi-nated materials with hierarchical microstructure for structural and functional applications.
- Atomic scale chemical and defect analysis in semiconducting nanowires with a correlation to the functional properties (Fig. 10).

Nanotribology (S. Brinckmann)

Group mission. The microstructure evolution during friction and wear is at the heart of this research group. The projects research the tribological behaviour on the micrometer scale to fundamentally understand the irreversible mechanisms that result in the energy and structural loss. The investigated evolution processes include grain refinement, plasticity especially at the surface, phase formation and dissolution. In addition to the microstructural formation, a constant focus of our research is an in-depth understanding of the friction coefficient and wear rate at the micrometer scale and the controlling mechanisms. Although we mainly focus on the dry contact of metals with an infinitely hard micrometer asperity, some projects probe the metal on metal contact in the presence and absence of lubricants. The initial and evolving surface roughness is of significant importance at the micrometer-scale. The environmental control and environmental induced surface layer evolution is taken into consideration. Recently, we started to investigate the effects of hydrogen on plasticity and fracture during tribology.

Research progress. In 2014 a nanoindenter Agilent/Keysight G200 was purchased, which allows to measure tangential forces and the quantification of the friction coefficient at the micro- and nanometer length scale with the addition of the nano-vision stage (see also “New Scientific Laboratories and Facilities”, “Nanoindentation and -tribology Laboratory”). In combination with the physical setup of the laboratory, methods for surface preparation, scratch testing and post-deformation surface topography identification were optimized. One primary benefit of the nanotribology research are the high-throughput experiments: the scratch velocity, normal force and scratch repetition can be varied on a micrometer-sized area. Hence, all experiments are using the identical material and possibly identical crystal orientation. Moreover, the asperity radius and the counter material (see Fig. 11) can be varied on the same material and with the same lubricant.

We started a number of current research projects ranging from delamination testing of PtIr thin films on WC (cooperation with Dr. P.-P. Choi, MA-Department), Mo_2BC thin films on Si (cooperation with Prof. J. Schneider, RWTH Aachen, Prof. Scheu, “Nanoanalytics and Interfaces” at the MPIE) and High Entropy Alloy thin films on Si (cooperation with Dr. K.G. Pradeep and Prof. J. Schneider, RWTH Aachen) to hardness and Young‘s modulus determination of intermetallic phases in a collaboration within the SN-Department. Three primary research results are summarized below.

Elasticity and fracture during tribology. During scratching in austenite, we found that the elastic and plastic depth is given by the Hertz and hardness definition, respectively, both of which were developed for static indentation although scratching is a dynamic process [14]. We identified three domains of tribology at the micrometer scale: wear particles form for high normal forces and these wear particles lead to additional compliance; crystal orientation dependent plastic plowing dominates for medium normal forces; and the microstructure and phase distribution determine the friction at the low normal

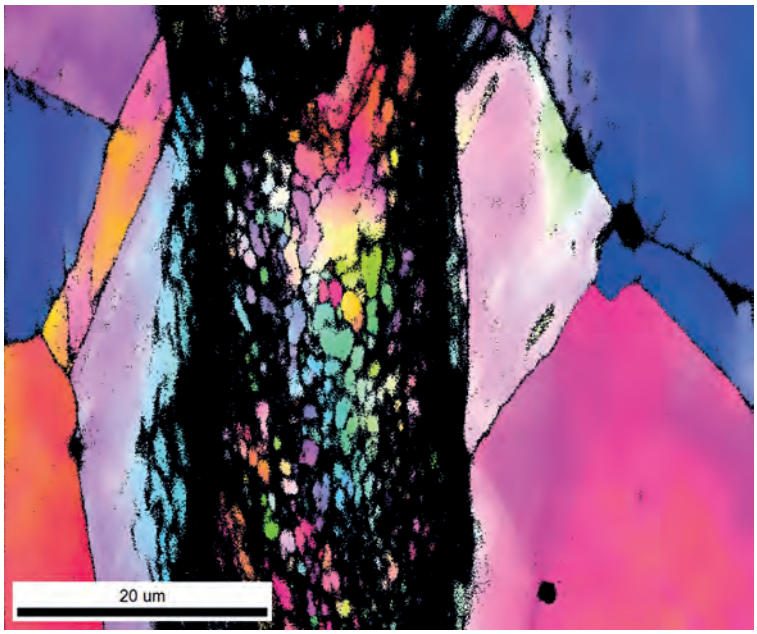

Fig. 12: *Grain refinement in coarse Cu after scratching. The scratch track is a fine-grained microstructure present after a single stroke scratch with a 20 µm indenter tip.*

forces [15]. Additionally, we observed crack formation and grain refinement (see Fig. 12) during single stroke experiments in other FCC metals.

Hydrogen embrittlement in nanotribology. We investigated the hydrogen embrittlement during tribology in Fe-Cr alloys, which were designed and produced in the MA-Department. To this end, we constructed a three-electrode electro-chemical cell for the G200. Initially, we investigated the pop-in behaviour during nanoindentation as a function of the electro-chemical charging and as a function of the grain orientation. During the scratching experiments, we observed that the surface roughness

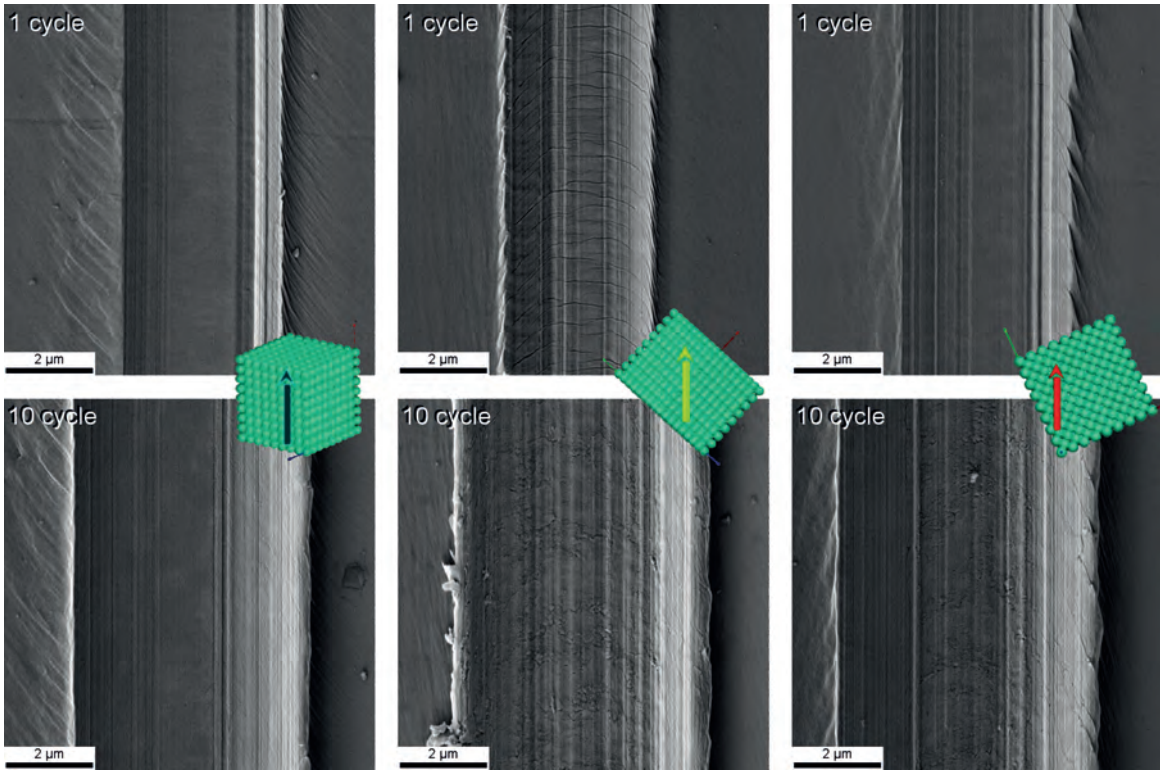

Fig. 13: *Single and repeating scratches in FeCr15 with 10 mN and 10 µm/s. The scratches are placed in different grain orientations. The center grain shows cracks already after the first scratch. After 10 cycles the scratch tracks significantly widened. In the center and right-hand image wear particles have developed.*

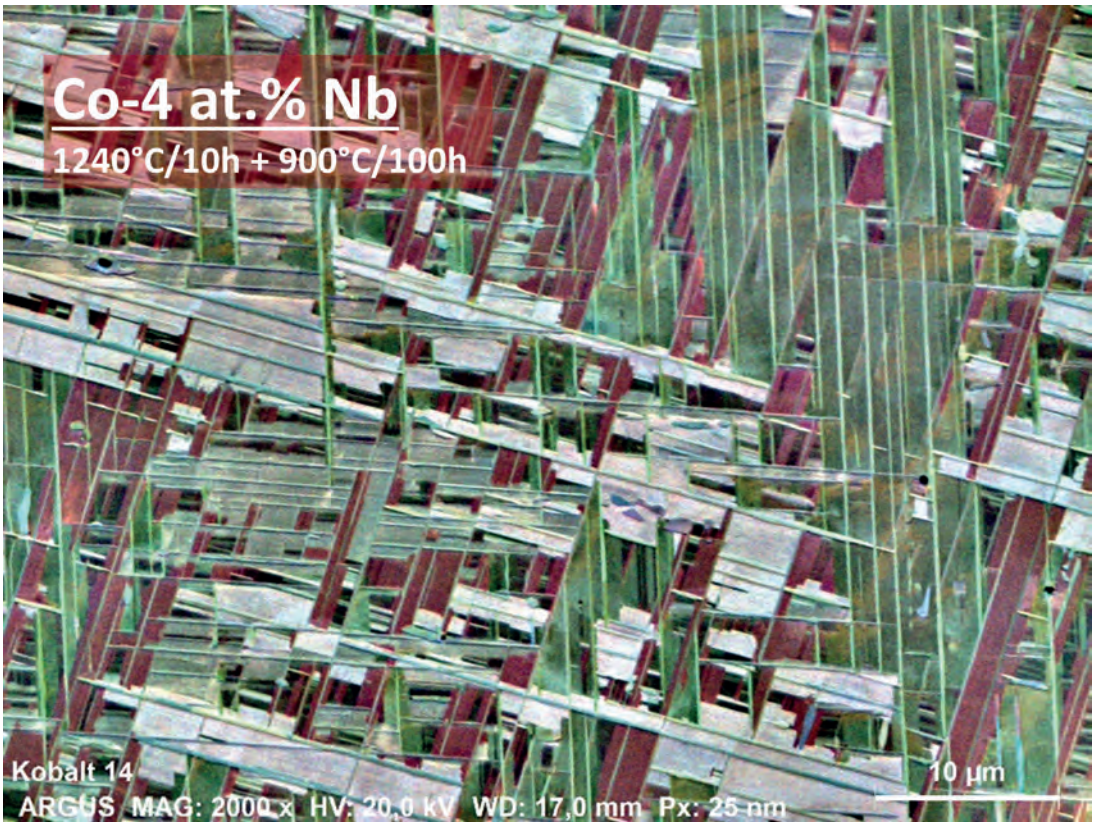

Fig. 14: *Widmanstätten-like morphology of needle-shaped intermetallic phase precipitation from super-saturated Co(Nb) solid solution. Different colours indicate different crystallographic orientations of the Co matrix. The picture was taken with a Zeiss Merlin SEM in FSD mode (image recorded by K. Angenendt).*

depends on the load order: initial scratching and subsequent polarization results in a rougher surface than initial polarization and subsequent scratching, as shown in Fig. 13.

Microstructure modifications. Most advanced bulk and thin film materials have a microstructure, which consists of fine and homogeneously distributed phases. The chemical and resulting microstructural stability is the key challenge in applying these materials in tribological applications, as friction and wear can lead to mechanical mixing and the introduction of dislocations, which would result in phase dissolution. We use pearlitic steel to study the stability of cementite and ferrite lamellae upon scratching. After scratching the surface, we investigate the microstructural stability on the surface and sub-surface in the material. In addition to investigating the tribological induced microstructure, we investigate the relation of phase boundary orientation on the friction and wear properties. With respect to pearlite, we investigate how the lamellae orientation determines the friction coefficient. The goal of this study is to fundamentally understand the friction behaviour of pearlite, which could lead to optimizing the microstructure to minimize friction and wear.

Intermetallic Materials (M. Palm, F. Stein)

Group mission. According to the Intermetallic Materials group´s mission, current research encompasses projects on fundamental aspects of phase stability and phase transformations of intermetallic phases as well as projects on establishing their properties in view of potential industrial applications. Most of the fundamental investigations are carried out in international collaborations while the more application-oriented projects are collaborations with industries.

Fundamental aspects of phase stability and phase transformations. Regarding alloy systems, the main focus of the group´s activities lies in research on iron aluminides. One of the unsolved fundamental questions in the Fe-Al system is the nature of the K-phase state (K for the German word ‘komplex’, which in this connection may be translated as ‘difficult’). The K-phase state exists between 250 and 400 °C and at Al contents between ~10 and 20 at.%, where a chemical structure occurs which shows an anomalous behaviour with respect to lattice parameters, electrical resistivity, magnetic properties and thermal dilatometry. This state was first described in 1950 and though it has been the topic of numerous investigations since then its exact nature is still unclear. With atom probe tomography

(APT) now a tool for direct observation of chemical order exists. In a collaboration with the Australian Centre for Microscopy and Microanalysis at the University of Sydney and the MA-Department at MPIE, well-defined samples were investigated by APT. Though the measurements did not reveal the existence of nano-sized, ordered regions/particles, the employed method of determining chemically sensitive, generalised multicomponent short-range order (GM-SRO) parameters by shell-based analysis of the three-dimensional atomic positions has general relevance for other alloy systems where quantitative chemical-structure evaluation of local atomic environments is required [26].

Also in the Fe-Al system, but for alloys with about 55 to 65 at.% Al, the eutectoid transformation Fe_5Al_8 (ε) ↔ FeAl + $FeAl_2$ has been studied [27-29]. This rapid solid-state reaction leads to very fine-scaled lamellar microstructures with average lamellar spacing of about 200 nm. In Ti-Al-based alloys, such microstructures lead to a combination of well-balanced properties in terms of creep, ductility and strength. However, there is limited knowledge about the properties of Fe-Al-based alloys in this composition range. Therefore, a series of as-cast as well as heat-treated alloys was analysed by SEM, electron-probe microanalysis (EPMA), XRD and differential thermal analysis (DTA). This ongoing research already led to an improved understanding of the composition dependence of all transition temperatures of the involved phases [27]. The coarsening behaviour of the lamellae at high temperatures is studied in detail and first results on the kinetics of this process are described on p. 151.

A combination of systematic experiments and calculations according to established theories for the interaction between solute atoms and dislocations has been performed to understand the strong solid solution hardening effect of V in Fe-Al. Comparison to Fe-Al-V-C alloys strengthened by V_8C_7 shows that a considerable volume fraction of carbide precipitates is needed for obtaining a comparable yield strength. However, such marked volume fractions of carbides are not desirable as they can lead to the formation of coarse, anisotropic shaped precipitates, which may act as sources for crack nucleation [30]. Also in view of the potential application of iron aluminide based alloys, the microstructure/property relationships of Fe-Al-Li and Fe-Al-Ti-B-(Mo,W) alloys have been established and the effect of Zr on the high-temperature cyclic oxidation behaviour of Fe_3Al-based alloys has been studied [31-33].

By thermal analysis (DTA and differential scanning calorimetry (DSC)), solidification behaviour and invariant reactions in a number of Fe-, Co- and Cr-based systems were studied [27,34-38]. Precise measurements of the solidus-liquidus intervals of

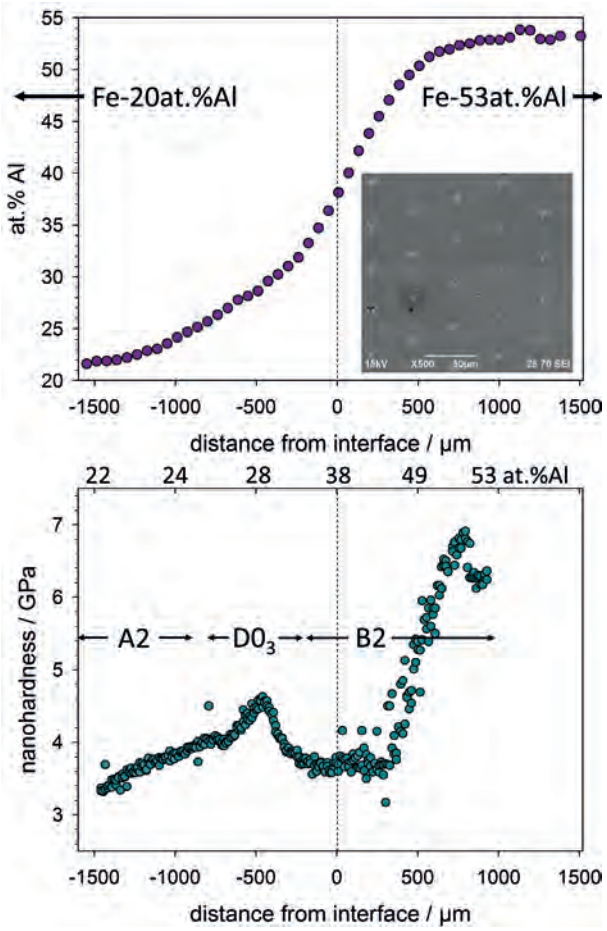

Fig. 15: *Composition dependence of the nanohardness of disordered Fe(Al) solid solution (A2) and its ordered variants $D0_3$ Fe_3Al and B2 FeAl as measured along a continuous concentration profile in a Fe-20at.%Al / Fe-53at.%Al diffusion couple. The micrograph shows an array of nanoindents in the diffusion zone.*

various steel types were performed by DTA/DSC and used as a basis for the development of an improved Scheil-Gulliver model to predict the solidification temperatures of steels [34]. Isothermal sections and liquidus surfaces of the ternary systems Fe-Al-Nb [35], Cr-Al-Nb [36], and Co-Si-Ti [37] were established by combining results from thermal analyses with phase analyses from EPMA and XRD.

Based on own extensive experimental results obtained within the inter-institutional Max Planck Society research initiative ''The Nature of Laves Phases'' and critically assessed literature data the systems Co-Al, Co-Nb, Al-Nb and Co-Al-Nb were thermodynamically modeled by the Calphad method [38,39]. Two-sublattice models were used for the three Laves phase polytypes – hexagonal C14 and C36 and cubic C15 – to enable a realistic description of their homogeneity ranges in the Co-Nb and Co-Al-Nb systems. The Al-Nb and Co-Al systems were re-assessed for a better description of the homogeneity ranges of Nb_2Al and B2 CoAl, respectively. The comparison between calculated and

experimental values shows that the optimized set of thermodynamic parameters gives a complete and consistent thermodynamic description of the whole Co-Al-Nb system [39].

Besides phase equilibria, also the kinetics of phase transformations and precipitation is a topic of the group. As an example, Fig. 14 shows the discontinuous precipitation of a complex intermetallic phase (whether this is monoclinic Co_7Nb_2 or hexagonal C36-type $NbCo_2$ Laves phase still has to be clarified) from a supersaturated Co solid solution. The binary Co-4at.%Nb alloy first was solution heat-treated for 10 h at 1240 °C to obtain single-phase fcc Co solid solution, and then hold at 900 °C for 100 h outside of the single-phase field to observe the discontinuous precipitation reaction.

Properties and application of intermetallics. Another focus of the group's work lies on studying the composition dependence of mechanical properties of intermetallic phases. In order to get well-defined and well-comparable, single-phase and single-crystalline material, diffusion couples are prepared from different metals or intermetallic phases and various micromechanical tests are planned to be performed along the concentration profiles obtained in the resulting diffusion zones. A first result of this ongoing project is shown in Fig. 15. By contacting pieces of Fe-Al alloys with 20 and 53 at.% Al at 1000°C for 100 h and slow cooling to room temperature, an extended continuous Al concentration profile has been obtained including the composition ranges of the disordered A2 Fe solid solution and the $D0_3$- and B2-ordered intermetallic phases Fe_3Al and FeAl. With the help of the nanotribology group, nanohardness measurements were performed along the concentration gradient. In the disordered A2 Fe(Al) composition range, the effect of solid solution hardening is clearly visible. As soon as the $D0_3$-type Fe_3Al phase occurs, a stronger increase in hardness is observed related to the effect of ordering. Within the composition range of the B2 FeAl phase, another very strong increase in hardness occurs. As the B2 FeAl phase is well known for its high vacancy concentration leading to strong vacancy hardening, the observed nanohardness increase can be expected to be related to the high density of vacancies. More detailed studies on that are ongoing.

As iron aluminides are considered as an economic replacement for stainless steels, their industrial manufacturing and evaluation of the resulting properties has become an important research topic. Within various collaborations with industries the casting of large brake discs for windmills, the rolling of different products and the forging of compressor blades has been investigated. It has also been shown that additive layer manufacturing (ALM) of iron aluminide based alloys by selective laser melting (SLM) and laser metal deposition is feasible [40]. Furthermore, in bi-lateral projects with industries, single-phase materials of the Al-rich Cu-Al intermetallic phases have been synthesised and characterised to establish fundamental physical properties, and phase equilibria in the Nb-based, high-melting Nb-Al-Fe systems are established.

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Research Projects in Progress

Nano-/Micromechanics of Materials (C. Kirchlechner)

Balila, Kirchlechner, Dehm: Reliability of fracture toughness test geometries at the micron-scale

Balila, Kirchlechner, Dehm: Deformation and fracture of interfaces in metallic materials

Balila, Kirchlechner, Dehm (in cooperation with M. Köhler, D. Raabe, MA-Department; J. Schneider, D. Music, V. Schnabel, RWTH Aachen): Fracture behavior of metallic glass thin films

Balila, Kirchlechner, Dehm (in cooperation with J. Michler, EMPA Thun, Switzerland): High temperature fracture mechanics

Davydok, Kirchlechner: Dislocation-grain boundary interaction studied by X-ray µLaue diffraction: The role of stacking fault energy

Djaziri, Kirchlechner, Dehm (in cooperation with J. Schneider, RWTH Aachen): Measuring fracture strain of Mo_2BC

Djaziri, Kirchlechner, Dehm (in cooperation with Y.J. Li, D. Raabe, MA-Department; S. Goto, Akita University, Japan): Shedding light on nanostructured pearlitic steel by advanced X-ray characterization

Kirchlechner: Micron-sized cantilevers and the Bauschinger effect

Kirchlechner (in cooperation with G. Pharr, UT Knoxville, TN, US): Probing dislocation grain-boundary interaction(s) by indentation pop-in statistics

Malyar, Dehm, Kirchlechner (in cooperation with J.-S. Micha, CEA-Grenoble): Dislocation slip transfer in micron-sized bi-crystals analyzed by advanced *in situ* methods

Marx, Kirchlechner, Dehm (in cooperation with M. Cordill, Erich Schmid Institut für Materialwissenschaft, Leoben, Austria): Temperature effects on the mechanical behavior of single and multilayer thin films on flexible substrates

Philippi, Kirchlechner, Dehm: Thermo-mechanical investigation of solder joints

Raghavan, Dehm (in cooperation with C. Tasan, MA-Department): Electroplasticity in metals

Raghavan, Harzer, Dehm: Plasticity of co-evaporated and sputtered multi-layered copper-chromium film

Raghavan, Kirchlechner, Dehm (in cooperation with M. Feuerbacher, FZ Jülich): Plasticity in fcc high entropy alloys

Soler, Harzer, Kirchlechner, Dehm (in cooperation with P. Mayrhofer, M. Bartosik, TU Wien, Austria): Role of bi-layer period on the mechanical response of a CrN / TiN multilayer

Soler, Harzer, Venkatesan, Kirchlechner, Liebscher, Dehm: Mechanical response of colloidal gold particles studied *in situ* in the TEM

Soler, Venkatesan, Dehm (in cooperation with several companies within the ENIAC Joint Undertaking EPPL): Global and local fracture properties of interfaces at variable temperature for robust material combinations in power devices

Subramanian, Kirchlechner: Algorithms for investigating satellite peaks in Laue patterns

Taniguchi, Kirchlechner, Liebscher, Dehm: Dislocation-precipitate interaction mechanisms

Advanced Transmission Electron Microscopy (C. Liebscher)

Harzer, Liebscher, Scheu, Dehm (in cooperation with T. Dennenwaldt, Interdisciplinary Center for Electron Microscopy, Ecole polytechnique fédérale de Lausanne): Electron energy loss spectroscopy of bcc-Cu in Cu-Cr thin film structures

Harzer, Djaziri, Raghavan, Dehm: Nanostructure, chemical composition, and mechanical properties of Cu-Cr thin film structures

Liebscher, Dehm: TEM investigation of sulfur segregation in Cu grain boundaries

Peter, Kirchlechner, Liebscher, Dehm: Dislocation grain boundary interaction in Cu grain boundaries studied by *in-situ* TEM

Soler, Venkatesan, Kirchlechner, Liebscher, Dehm: *In-situ* TEM deformation studies on nanoparticle systems

Stoffers, Cojocaru-Mirédin, Liebscher, Raabe, Scheu, Dehm: Atomic structure of segregation effects at grain boundaries in multicrystalline silicon

Venkatesan, Soler, Dehm: Global and local fracture properties of interfaces and their correlation to microstructure in electronic power devices

Venkatesan, Liebscher, Scheu, Dehm (in cooperation with P. Krogstrup, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Denmark): Atomic scale chemical and defect structure investigation of MBE grown III-V semiconducting nanowires

Nanotribology (S. Brinckmann)

Brinckmann, Dehm: Nanotribology in austenite and copper

Duarte Correa, Brinckmann, Dehm: Crystallization kinetics and microstructural evolution of metallic glasses

Duarte Correa, Brinckmann, Dehm: Corrosion and wear at the nanoscale

Fink, Brinckmann, Dehm: Nanotribology of iron-alloy microstructures

McKeown, Brinckmann, Dehm: Nanoscratch-testing of thin films

Intermetallic Materials (M. Palm, F. Stein)

Azmi, Michalcová, Palm: Microstructure and mechanical properties of Fe–Al–Nb–B alloys

Li, Stein (in cooperation with A. Scherf, M. Heilmaier, KIT Karlsruhe): Al-rich Fe–Al *in-situ*-composite materials: microstructure and mechanical properties

Li, Stein (in cooperation with R. Spatschek, CM-Department): Coarsening kinetics of fine-scaled lamellar B2-FeAl + $FeAl_2$ eutectoid microstructures

Lotfian, Prokopčáková, Švec, Palm (in cooperation with Leistritz Turbinenkomponenten Remscheid GmbH; IST RWTH Aachen; Access e.V.): Forged iron aluminide turbine blades: Process development and characterisation

Luo, Kirchlechner, Dehm, Stein: *In-situ* micromechanical studies of intermetallic phases along concentration profiles in diffusion couple zones

Marx, Palm (in cooperation with Winterthur Gas & Diesel Ltd.; Wärtsila Finland Oy; Wärtsila Netherlands BV; Kennametal Stellite GmbH; ABB Turbo Systems AG): Intermetallics for engine applications

Michalcová, Senčeková, Szczepaniak, Palm (in cooperation with Airbus Group Innovations; Siemens AG Corporate Technology; Fraunhofer-Institut für Lasertechnik; Dr. Kochanek Entwicklungsgesellschaft; NANOVAL GmbH & Co. KG): RADIKAL – Alloy development for and characterisation of iron aluminide components manufactured by additive layer manufacturing

Palm (in cooperation with P. Kratochvíl, J. Pešička, R. Král, Dept. Physics of Materials, Charles University Prague; M. Švec, Technical University Liberec): Basic principles of solid solution hardening in iron aluminide alloys

Palm, Stein (in cooperation with R. Wartbichler, S. Mayer, H. Clemens, Montanuniversität Leoben, Austria): The effect of Mo additions and processing on the microstructure of Al-rich Ti–Al alloys

Poková, Liebscher, Stein: TEM studies on dislocations and deformation mechanisms of Laves phases

Stein (in cooperation with A. Kaiser, Fraunhofer IKTS, Dresden): High-temperature phase equilibria and melting behavior of Nb-rich Fe–Al–Nb alloys

Stein (in cooperation with T. Horiuchi, Hokkaido University of Science, Japan): Kinetics of peritectoid decomposition reactions

Stein (in cooperation with T. Horiuchi, Hokkaido University of Science, Japan): Discontinuous precipitation of intermetallic phases from Co solid solution

Stein, Li, Liebscher (in cooperation with A. Szczepaniak, H. Springer, MA-Department; H. Becker, T. Zienert, A. Leineweber, TU Bergakademie Freiberg): Substructure formation and crystallographic transformation of the complex intermetallic phase Fe_2Al_5

Varona Caballero, Palm (in cooperation with S. Milenkovic, IMDEA Materials): Development of new generation NiAl-based eutectic composites with tuneable properties

PART III.

INTER-DEPARTMENTAL RESEARCH ACTIVITIES – SELECTED HIGHLIGHTS

Ductile Mg Alloys by Combining *ab initio* and Experimental Methods

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Magnesium based alloys are attractive for structural applications owing to their low mass density, good castability and efficient recyclability [1, 2]. However, wider application of sheet Mg is hindered by its poor room temperature formability, which is caused by pronounced basal slip and a strong basal-type texture [1, 2]. According to this, the von Mises' criterion for five independent deformation modes to satisfy an arbitrary shape change cannot be met. In hcp crystals strain along the crystal c-axis can only be accommodated by the activation of non-basal slip and deformation twinning, fulfilling the von Mises' criterion requires the activation of non-basal dislocation slip. We showed that single-phase solid-solution Mg-Y alloys exhibit an increased room-temperature ductility by about 5 times, while maintaining a comparable strength and a well-balanced work hardening [1].

We showed by joint transmission electron microscopy (TEM) measurements and *ab initio* calculations that the ductility increase in Mg-Y alloys is caused by an increased activity of <c+a> dislocation slip [2]. This facilitated activation of out-of-basal-plane shear modes through the addition of Y to Mg is correlated to a significantly decreased I_1 intrinsic stacking fault energy (I_1 SFE) [2]. Here, the I_1 SFE is decreasing with increasing Y concentration. We propose that this reduction of the I_1 SFE can be used as a guiding parameter (among others) connected with the ductility increase in the Mg-Y system acting as follows: The enhanced ductility is caused by a high activity of pyramidal <c+a> dislocations as slip modes out of the basal plane. The nucleation of <c+a> dislocations is the critical step in providing out-of-basal-plane shear. This is associated with the SFI_1: the sessile SFI_1, whose energy decreases with Y alloying, is bound by a pyramidal partial dislocation. This dislocation arrangement enables the formation of dislocation structures on pyramidal planes. In line with the nucleation source configuration studied by Yoo et al. [3] we suggest that the SFI_1 acts as heterogeneous nucleation source for pyramidal <c+a> dislocations. Consequently, the observed (TEM) and calculated (*ab initio*) reduced I_1 SFE through the addition of Y could cause the formation of stable SFI_1 in Mg-Y alloys and hence, provide sources for <c+a> dislocations. The reduced SFE leads then to a higher probability of formation of SFI_1 nucleation sources and therefore higher ductility.

We now used the I_1 SFE of Mg-X solid solutions more systematically as a guiding parameter for the design of a general class of ductile Mg alloys (Fig.1). Based on *ab initio* predictions of these I_1 SFE, promising alloys, i.e. those characterized by a reduced I_1 SFE, were produced, homogenized, rolled, mechanically tested and characterized regarding their microstructure, deformation mechanisms and I_1 intrinsic stacking fault energy and we experimentally confirmed that alloys with theoretically predicted decreased I_1 SFE indeed possess significantly enhanced room temperature ductility and experimentally observed increased <c+a> dislocation slip and decreased I_1 intrinsic stacking fault energies [4] (Fig. 2).

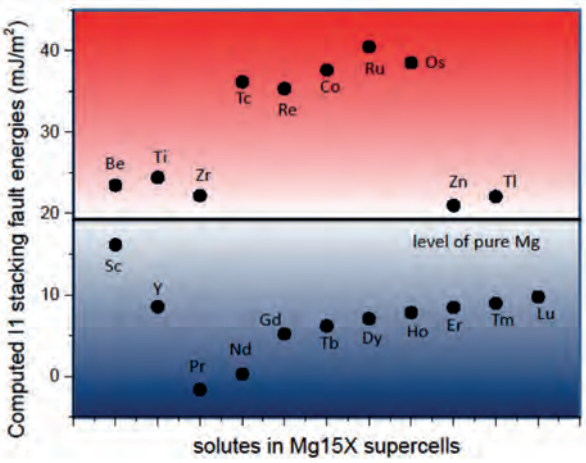

Fig. 1: *Ab initio predicted values of I_1 SFE in binary Mg-X alloys.*

To allow a fast solute assessment without lengthy explicit *ab initio* calculations, we analyzed the correlations and anti-correlation between the I_1 stacking fault energy and intrinsic materials parameters. Our analysis reveals that the atomic volume of pure solutes, their electronegativity and bulk modulus are related to the I_1 SFE. To compare the impact of solutes on the I_1 SFE with that of yttrium we introduced a numerical quantity, the 'Yttrium Similarity Index' which is based on these interrelations and gives the change of the I_1 SFE in Mg alloys with respect to Mg-Y [5]. When considering only binary Mg alloys, we hardly found any alternative solutes providing similar I_1 SFE reduction as that due to rare-earth (RE) additions. Therefore, we extended the 'Yttrium Similarity Index' to ternary Mg

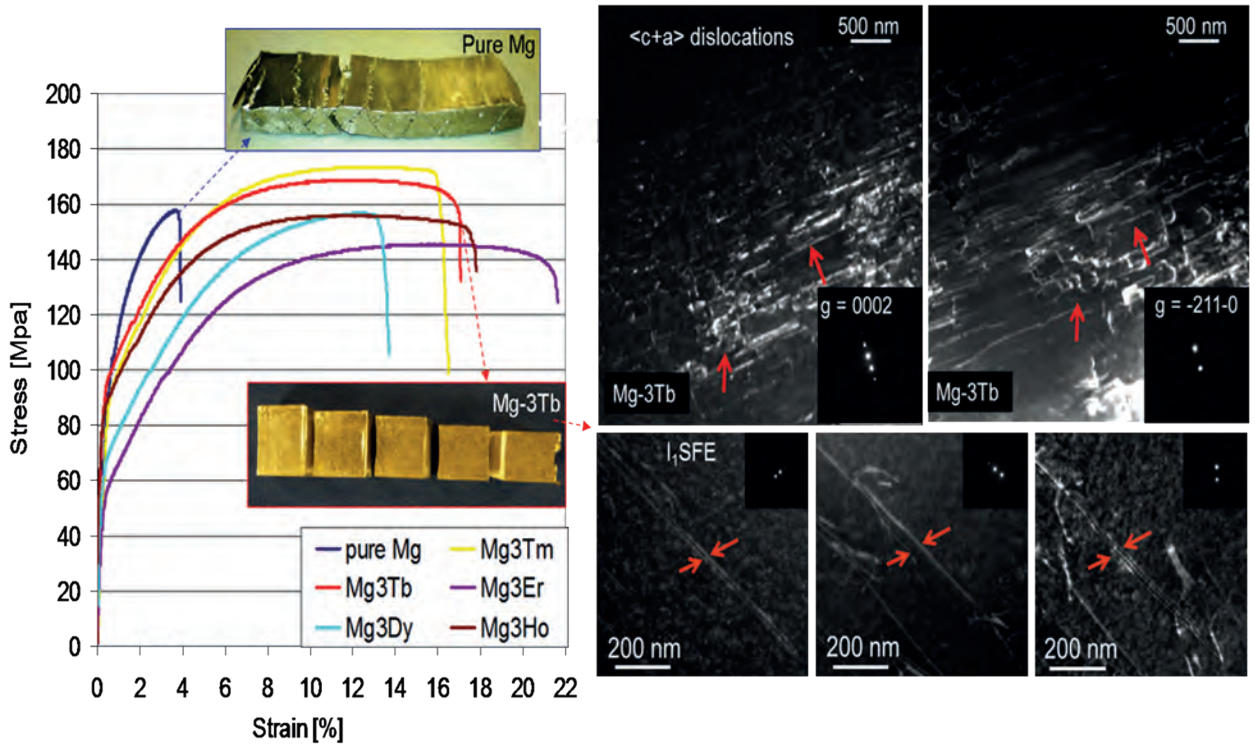

Fig. 2: *Tensile stress-strain (eng. strain) of the newly designed Mg alloys in as-homogenized conditions in comparison to pure Mg. The optical photographs show the alloys after cold rolling to different thickness reductions. The dark-field TEM micrographs show increased activity of <c+a> dislocations (upper micrographs) and reduced I_1 SFE in the new alloys.*

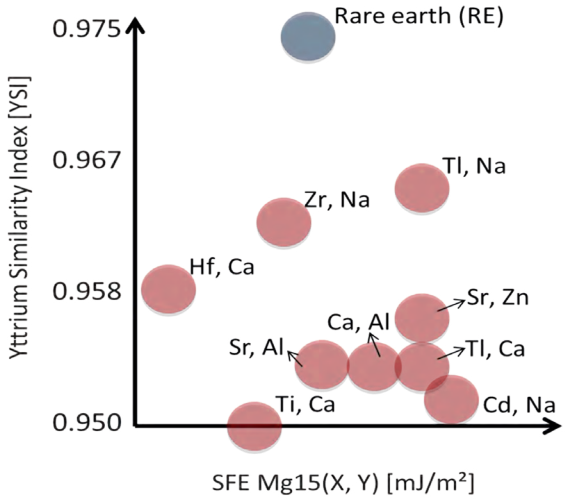

Fig. 3: *Yttrium Similarity Index (YSI) and ab initio calculated stacking fault energy (SFE) for $Mg_{15}(X, Y)$ (X, Y – alloying elements) of promising ternary alloys; for comparison the YSI and SFE for rare earth elements are also shown.*

alloys (Fig. 3). Quantum-mechanical calculations have been subsequently performed for 11 solute pairs with YSIs higher than 0.95 and they were all found to reduce I_1SFE in excellent agreement with the prediction based on the 'Yttrium Similarity Index' [5]. Our future alloy design strategy is based on the synthesis and characterization of these new ternary *ab initio* guided alloys.

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Design of Strong and Tough Metallic Glasses: Beyond Poisson's Ratio

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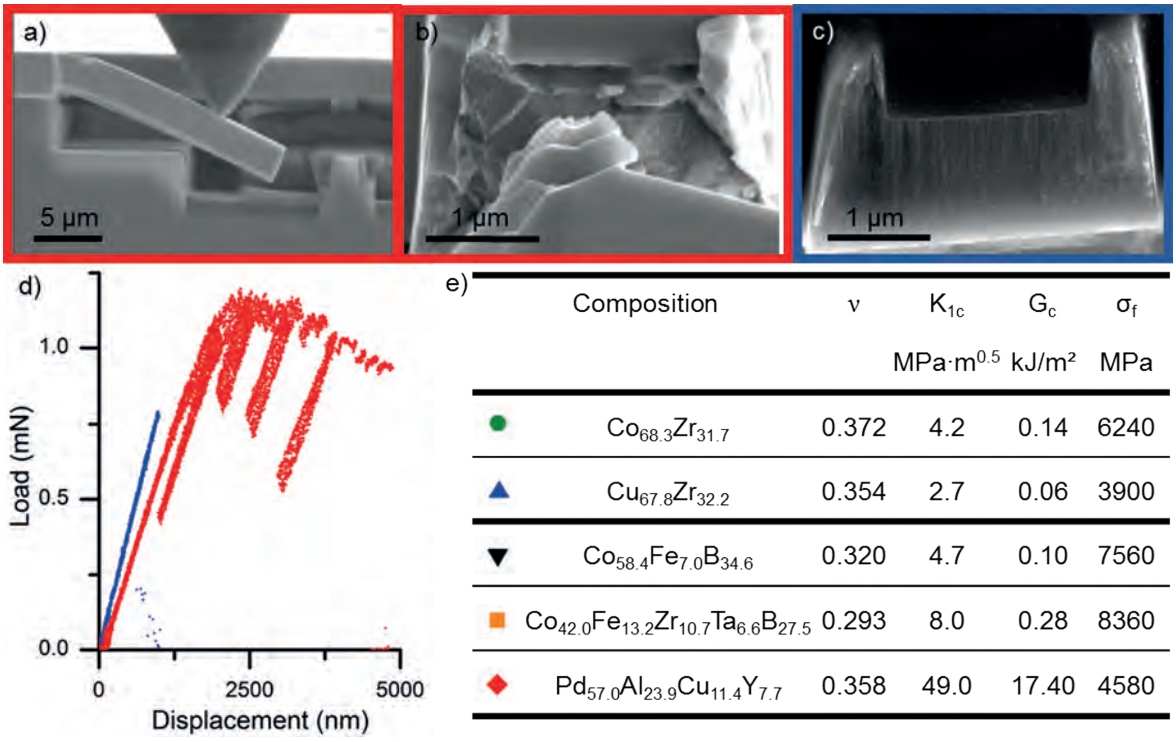
Metallic glasses (MGs) are becoming increasingly attractive due to their outstanding mechanical and soft-magnetic properties. Co-based MGs, e.g., exhibit a fracture strength above 5 GPa and an elastic modulus of more than 260 GPa [1]. Hence, these materials attract high interest.

Although MGs have been studied for the last decades, they have been mostly developed by using empirical glass-forming rules [1], suggesting a critical Poisson's ratio above which all metallic glasses exhibit pronounced toughness [2, 3]. However, several exceptions to this rule were recently observed [4, 5].

Reaching beyond this approach we established a fundamental criterion, based on chemical bonding, to design fracture resistant MGs. Through correlative *ab-initio* molecular dynamics (MD) simulations based on density functional theory and micro-scale fracture testing, conducted *in-situ* in a scanning electron microscope on magnetron sputtered metallic glass thin films, we are now able to explain the deviations from the concept of Poisson's ratio using ν to predict the brittle-ductile transition in MGs [3]. For that purpose we have simulated, synthesized and tested 5 different compositions (2 binary, 1 ternary, 2 multi-component MGs).



e)

Composition	ν	K_{1c} MPa·m$^{0.5}$	G_c kJ/m²	σ_f MPa
● $Co_{68.3}Zr_{31.7}$	0.372	4.2	0.14	6240
▲ $Cu_{67.8}Zr_{32.2}$	0.354	2.7	0.06	3900
▼ $Co_{58.4}Fe_{7.0}B_{34.6}$	0.320	4.7	0.10	7560
■ $Co_{42.0}Fe_{13.2}Zr_{10.7}Ta_{6.6}B_{27.5}$	0.293	8.0	0.28	8360
◆ $Pd_{57.0}Al_{23.9}Cu_{11.4}Y_{7.7}$	0.358	49.0	17.40	4580

Fig. 1: *[6] In-situ micro-cantilever fracture experiments. The fracture strength and toughness of the metallic glass thin films are measured by employing both un-notched and pre-notched specimens. a) Representative scanning electron image of an in situ micro-cantilever deflection experiment performed on a $Pd_{57.0}Al_{23.9}Cu_{11.4}Y_{7.7}$ glass. b) and c) show high magnification images of the crack trajectory and fracture surface of the tough $Pd_{57.0}Al_{23.9}Cu_{11.4}Y_{7.7}$ and the brittle $Cu_{67.8}Zr_{32.2}$ metallic glass, respectively. d) Load-displacement graphs for the brittle $Cu_{67.8}Zr_{32.2}$ in blue and the tough $Pd_{57.0}Al_{23.9}Cu_{11.4}Y_{7.7}$ in red. The dissipated energy before fracture (area under the curve) for the highly damage tolerant $Pd_{57.0}Al_{23.9}Cu_{11.4}Y_{7.7}$ glass is much higher compared to the brittle $Cu_{67.8}Zr_{32.2}$ glass. e) Summary of the ab initio calculated Poisson's ratio (ν), and the measured quantities fracture toughness (K_{1c}), fracture energy (G_c) and fracture strength (σ_f) of the glasses studied within this work. Fig.1 summarizes these results for the five glass compositions tested. Further microstructural characterization has been undertaken, including transmission electron microscopy and atom probe tomography (APT) to establish the homogeneity and confirm the amorphous nature of these samples. The combination of theoretical (ab initio MD) and experimental (mechanical and microstructural characterization) reveal that the fraction of bonds stemming from deep core, hybridized states compared to the overall bonding defines damage tolerance in glasses.*

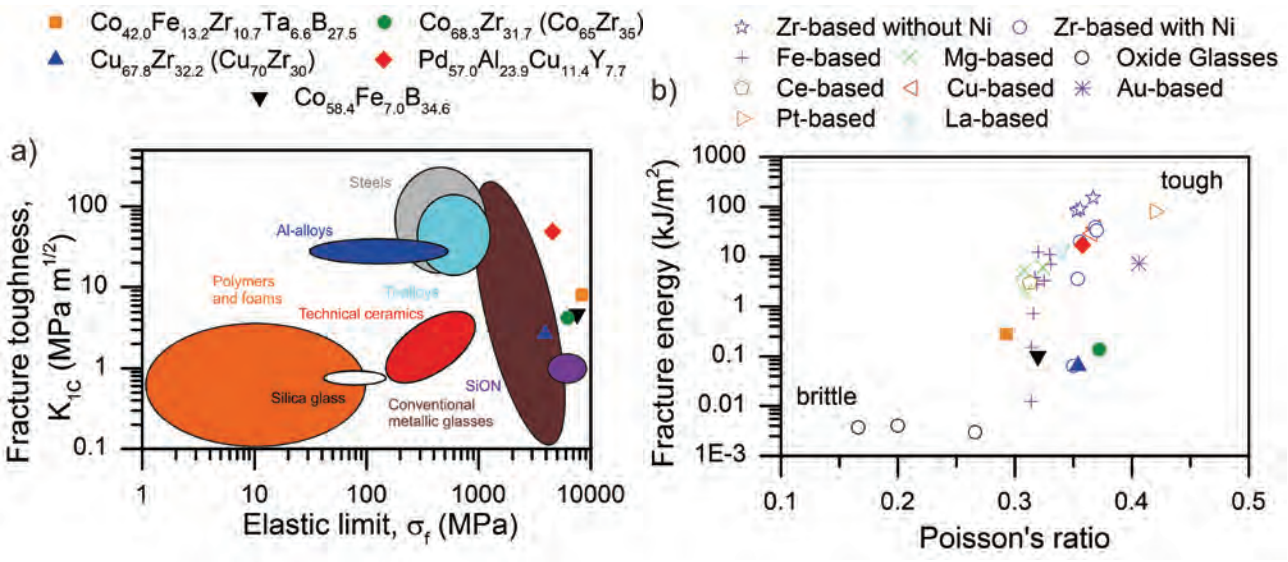


Fig. 2: *[6] Experimental validation reveals extraordinary damage tolerance for the metallic glasses studied in this work. a) The fracture strength of the glasses studied in this work is close to the ideal strength of the material. The $Pd_{57.0}Al_{23.9}Cu_{11.4}Y_{7.7}$ thin film metallic glass is identified to exhibit high damage tolerance. b) Poisson's ratio cannot gauge the chemical origin of the rapid evolution from brittle to tough behaviour. Literature data for the Mg-based, Ce-based and La-based [7, 8], Fe-based [9], oxide glasses [2, 10], Zr-based [4, 11], Cu-based [12, 13], Pt-based [14] and Au-based [7] glasses are presented. Fig. 2 compares the mechanical behaviour of the glasses that we developed with other known metallic glasses in an Ashby-type map. By investigating the bonding states of the different MGs via electronic density-of-states analysis we reveal the different bonding behaviour. The tough Pd-based glass e.g. shows low hybridization (Pd-Al) in contrast to the brittle CuZr glass which shows a strong hybridization while having a similar poisson's ratio. Therefore, bond hybridization is identified as a suited indictor for damage tolerance of MGs. Our approach allows for searching novel damage tolerant glasses by screening the electronic structure of yet new chemical compositions.*

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Initial Wear: Engineering down to the Atomic Scale

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With the quickly growing demand for high quality optical lenses glass molding (PGM) is a pivotal manufacturing method. This modern technology enables effective, replicative and large-scale fabrication of complex shape optics such as aspherical or diffractive lenses and lens arrays (Fig. 1) without any grinding and polishing steps.

As shown in Fig. 1, during the PGM process, glass blanks are placed in the mold of a pressing tool and are heated under vacuum or N_2 protective atmosphere up to the glass forming temperature, which normally ranges from 400 to 700°C. Subsequently, high press forces (2-20kN) are applied for several minutes until the mold form is homogeneously filled with glass. After controlled cooling, the final products can be detached from the mold. Since the molds experience not only thermo-mechanical stresses but are also subjected to a severe thermochemical environment, detrimental oxidation and corrosion processes finally lead to severe problems such as glass sticking. This phenomenon usually occurs after numerous cycles, limiting the lifetime of the molds, and is a decisive factor for economical industrial production of high-precision glass molds [1, 2].

The aims of the project Initial Wear are to investigate the fundamental mold degradation mechanisms, in particular in their initial stages. Degradation is studied using (sub-) nanometer scale characterization methods to propose a model, based on which the service lifetime of the molds can be predicted and even prolonged.

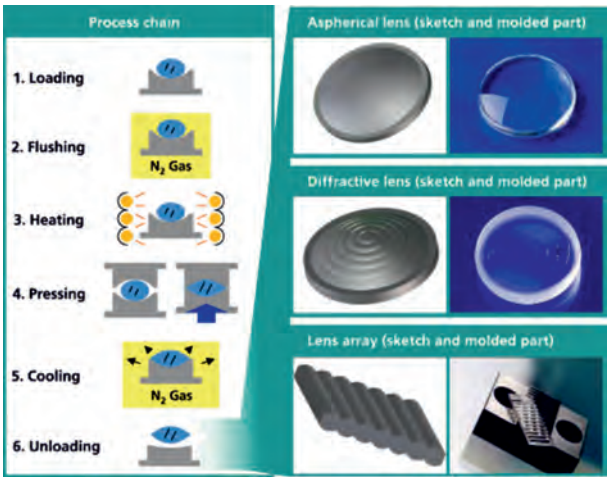

Fig. 1: *Outline of the precision glass molding process and the pictures of the representative products (image taken from IPT).*

In this research, the studied mold material is ultrafine grained (average grain size is around 200 nm) WC/Co hard mental with a sputter-deposited $Pt_{0.3}Ir_{0.7}$ coating, which is reported to be one of a most promising material system for PGM application [3]. High

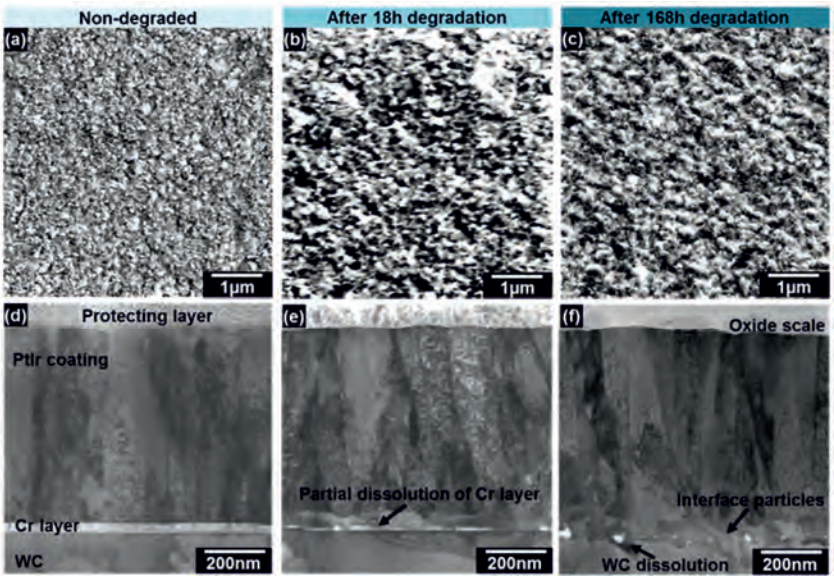

Fig. 2: *SEM images taken from the specimen surface (a-c) and TEM images taken from the specimens' cross section (d-e). (a) and (d) for the non-degraded specimen, (b) and (e) for the 18 h degraded specimen and (c) and (f) for the 168 h degraded specimen.*

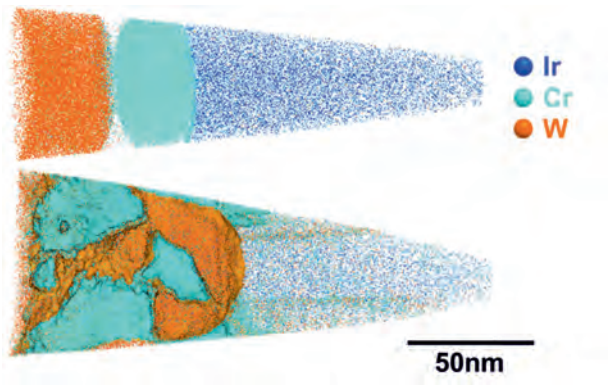

Fig. 3: APT elemental maps for the non-degraded specimen (upper) and the 168 h degraded specimen (lower).

adhesive strength between the top coating, which mainly serves to avoid sticking of glass to the hard metal, and the hard metal is necessary to avoid coating delamination, therefore an adhesive Cr interlayer is normally deposited [4].

Four main parameters influence the mold degradation processes, namely: atmosphere, temperature, mechanical stress and glass composition. The effects of atmosphere and elevated temperature are investigated because these two factors are common to all the PGM production techniques and seem to be the main factors controlling mold degradation. Therefore, specimens were firstly degraded for different exposure times under a well-controlled condition (temperature: 630°C, atmosphere: N_2/2.5%H_2 gas mixture with oxygen partial pressure of $1.23*10^{-23}$ bar), where the conditions are typical of real PGM processes. After degradation, different methods were used to characterize the specimens. Scanning electron microscopy (SEM) was applied to examine the surface morphology and damages; transmission electron microscopy (TEM) was employed to reveal the specimen microstructure and atom probe tomography (APT), which is a powerful tool for the characterization of thin-film materials [5, 6, 7] as well as nanometer-thick oxide scales [8], was utilized to acquire the 3D chemical compositions of different regions of the specimens with near-atomic resolution.

Fig. 2 shows SEM images of the specimen surface and TEM images of the specimen cross section. After 18 h degradation, the Cr adhesive layer is mostly intact but already partially dissolved. Moreover, after 168 h degradation, the original Cr layer is replaced by a chain of nanometer-sized particles and localized dissolution of WC hard metal results in a rough interface. Besides, an oxide scale of about 100 nm in thickness can be found, which leads to the change of the surface topology.

APT results are shown in Fig. 3 and Fig. 4. Interdiffusion between the PtIr coating, Cr adhesive layer and WC substrate can be observed, which assist the formation of the Cr rich (26at.% Cr, 55at.% Ir and 19at.% Pt) and W rich (25at.% W, 60at.% Ir and 15at.% Pt) interface particles. At the same time W atoms and Cr atoms diffuse upward along the grain boundaries and triple junctions of the PtIr coating to its surface where they are subsequently oxidized. However, no oxidation was observed in the bulk, raising questions about how exactly the WC is degraded.

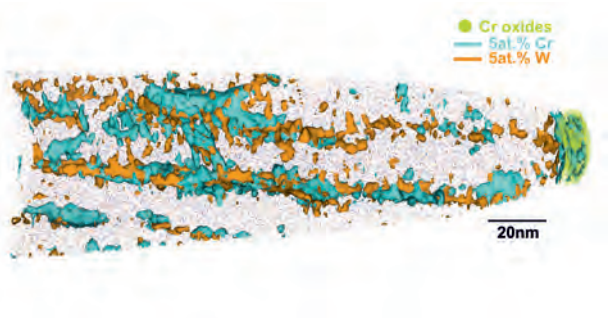

Fig. 4: *APT elemental map of the 168 h oxidized specimen.*

The experimental results achieved up to now clearly reveal degradation induced by atmosphere and elevated temperature. Further studies will focus on the effects of mechanical and chemical loads on surface degradation mechanisms.

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Towards Atomistically-Guided High Entropy Alloy Design

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In the past decade, the high entropy alloy (HEA) concept has attracted extensive research attention. This new alloy design strategy aims at the maximization of the entropy of mixing with the purpose of producing massive solid solution, single phase microstructures. The heavy lattice distortion and the thereby introduced sluggish diffusion are proposed to jointly contribute to high thermal stability and excellent mechanical properties. However, among various HEAs that have been designed according to this concept, most show brittle, multi-phase microstructures, and thus fail to prove the principle of the original concept described above. These unsuccessful design efforts raise concerns about the future applicability of HEAs. At the MPIE, various research projects have been initiated in the Adaptive Structural Materials group on this newly emerging field, taking off from the only alloy system that develops a single fcc solid solution upon conventional casting: the FeMnNiCoCr system. The main focus is on: (i) replacing currently adopted phenomenological criteria with physically-based alloy design guidelines based on density-functional-theory (DFT) *ab initio* simulations; (ii) designing novel, high performance HEAs that have the potential to replace alloys currently in service. Here a key focus is to revert to non-equiatomic alloy compositions to greatly expand the compositional ranges in search for potential future alloys (Fig. 1) [1].

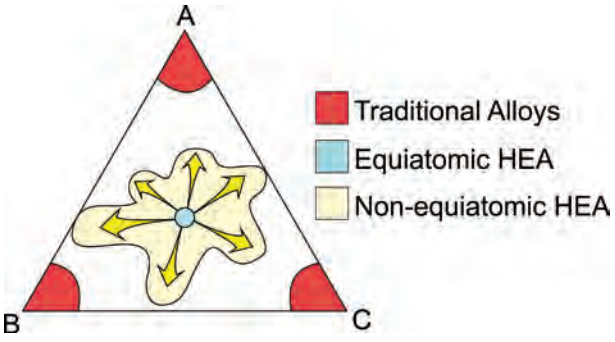

Fig. 1: *A schematic comparison of traditional alloys with one base element and minor alloying additions, high entropy alloys with equiatomic compositions of all alloying elements, and non-equiatomic - yet still massively alloyed - high entropy alloys, on the isothermal cross section of a ternary phase diagram [1].*

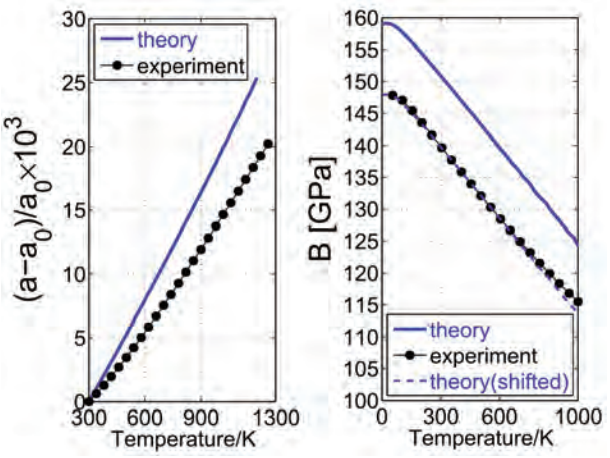

Fig. 2: *Calculated (solid blue lines)* ***(a)*** *thermal expansion and* ***(b)*** *isothermal bulk modulus as a function of temperature compared to experiment (black solid circles). The calculated thermal expansion and bulk modulus correspond to the fcc DLM phase and include all free energy contributions, i.e., electronic, vibrational, and magnetic. The dashed blue line in (b) is obtained by a constant shift of the calculated bulk modulus (blue solid line) to match the experimental bulk modulus extrapo*lated to T = 0 K. Figure taken from [2] with permission.

The description of entropic contributions from *ab initio* for multi-component magnetic alloys, such as e.g., FeMnNiCoCr, is a challenging task especially regarding finite temperature descriptions and increasing computational costs of supercell calculations. To cope with these challenges we have implemented and extended an integrated approach that is based on the exact-muffin-tin-orbitals approach to DFT in conjunction with the Debye model (for the vibrational degrees-of-freedom), the coherent potential approximation (for chemical disorder), the disordered local moment approach (for spin disorder) , and with a mean field approximation (for magnetic excitations). We have utilized this integrated *ab initio* approach to investigate in detail the phase stabilities of the hcp, fcc, and bcc phases in various magnetic states in the FeMnNiCoCr HEA [2]. The strength of the approach is demonstrated in Fig. 2 where we compare the computed thermal expansion and the bulk modulus (blue lines) of the thermodynamically most stable

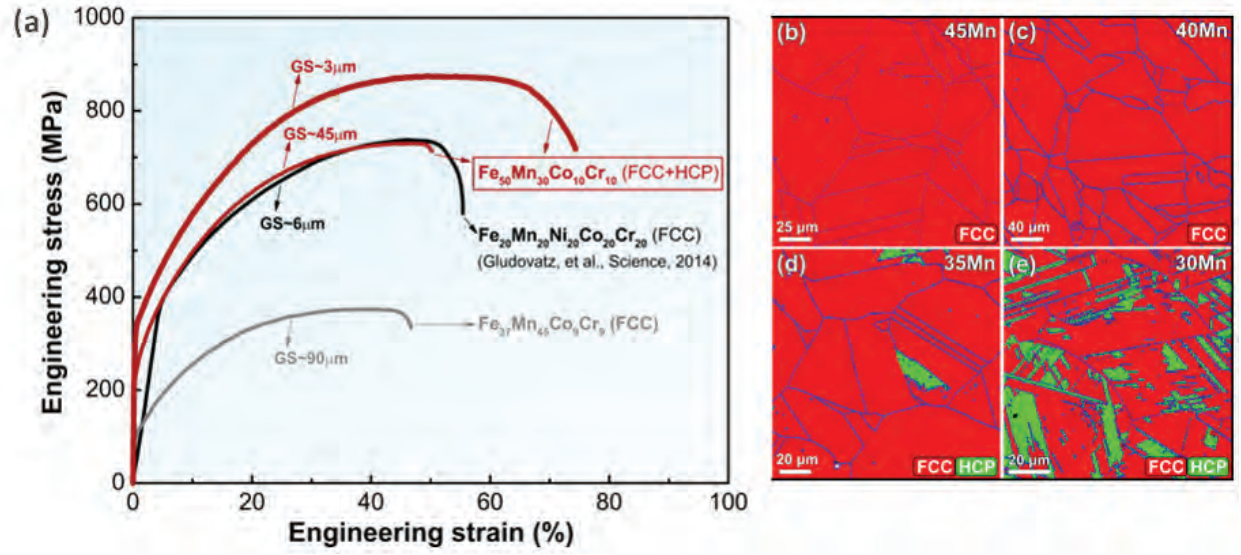

Fig. 3: (a) *Comparison of the mechanical behaviour of the TRIP-HEA and two single phase HEAs;* **(b-e)** *EBSD phase maps of $Fe_{80-x}Mn_xCo_{10}Cr_{10}$ (x = 45, 40, 35 and 30) HEAs demonstrating the increase in hcp% with decreasing Mn.*

phase, paramagnetic fcc, with experimental data (black dots). The developed toolbox enables confident investigations of quantities that are not easily accessible by experiment. We, e.g., recently demonstrated that entropy contributions other than the configurational one (vibrational, electronic, magnetic) are not negligible as previously assumed [2]. Furthermore, having these results available for the different phases (e.g. fcc and hcp), allows us to calculate the stacking fault energy (SFE) (using the ANNNI model) which is a critical quantity for plasticity and thus an important input to our experimental efforts.

Having access to theoretically determined SFE's as a function of composition, especially in such complicated alloy systems, is a strong support to our metallurgical alloy design process. In fact, our current experimental efforts clearly demonstrate that by optimizing SFE, properties much superior to presently proposed HEAs can be achieved. Fig. 3a shows one such clear example. The transformation induced plasticity (TRIP)-HEA $Fe_{50}Mn_{30}Co_{10}Cr_{10}$ developed in our group outperforms the equiatomic FeMnNiCoCr alloy in quasi-static tension test at room temperature. Similarly, we have observed that twinning induced plasticity (TWIP)-HEA $Fe_{40}Mn_{40}Co_{10}Cr_{10}$ has comparable mechanical properties to the FeMnNiCoCr alloy, despite the decreased alloying [4]. The accompanying microstructure characterization (Fig. 3b-e) reveals the critical role of Mn here in this four-component system, in both controlling the fraction of thermally-induced hcp martensite, and also the transition from dislocation plasticity to mechanically induced twinning and/or martensitic transformation assisted plasticity.

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Atomistic Understanding of the Off-Stoichiometry of κ-Carbides in Density Reduced Steels

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Fe-Mn-Al-C steels show excellent combination of strength, formability and low density rendering these materials attractive for light-weight vehicle applications [1-5]. The precipitation of nano-sized κ-carbides significantly strengthens these steels while preserving good ductility, owing to their excellent strain hardening [2, 3]. Though deformation mechanisms like glide plane softening, shear-band-induced plasticity (SIP) and microband-induced plasticity (MBIP) have been proposed [1, 4, 5], the interaction between dislocations and κ-carbides are still not well understood. The stress contribution from shearing of ordered particles is closely related to the antiphase boundary energy (APB) along the slip plane [6] and thereby to the stoichiometry and site-occupancy of the κ-carbides. Although it is known that κ-carbides tend to have off-stoichiometric composition, this matter has, owing to experimental challenges, hardly been experimentally quantified. Therefore, there is a lack of reliability of thermodynamic databases and a lack of understanding of the reasons for the off-stoichiometry. Here, we employ atom probe tomography (APT) to accurately determine chemical compositions and subsequently density functional theory (DFT) to predict the corresponding elemental site-occupancy in κ-carbides.

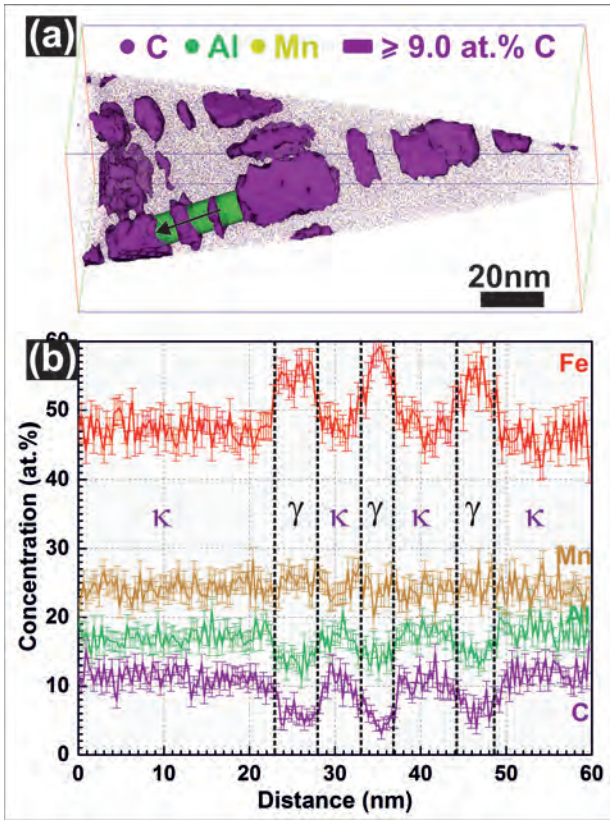

Fig. 1: *(a) 3D APT map showing κ-carbides, which are visualized by a 9 at.% C iso-concentration surface. (b) Elemental partitioning between κ-precipitates and γ-matrix along the cylindrical region of interest highlighted in green in (a).*

An austenitic Fe-29.8Mn-7.7Al-1.3C (wt%) steel is aged at 600°C for 24 hours to cause precipitation of coherent κ-carbides. Using a local electrode atom probe (LEAP) 3000X HR, the three-dimensional (3D) morphology of the nano-sized κ-carbides is revealed (Fig.1a). Cuboidal and plate-like κ-carbides are arranged in the form of stacks along three orthogonal directions which are elastically soft <001> crystallographic directions according to TEM observations [3]. There are two kinds of γ channels in different widths, broad ones of 10 - 40 nm in between particle stacks and narrow ones of 2 - 5 nm within particle stacks. Due to projection effects, particles of cubic shape in common TEM observations might actually have a much smaller size in the third dimension, i.e. plate-like shape. Al and C atoms clearly partition into the κ-carbides from the γ-matrix; no compositional difference is noticed between bigger cuboidal and smaller plate-like ones (Fig.1b). Their average chemical compositions are determined by careful mass spectrum analysis (Table 1). Instead of the ideal $L'1_2$ stoichiometry $(Fe, Mn)_3AlC$, the measured composition of $Fe_{2.0}Mn_{1.1}Al_{0.9}C_{0.6}$ indicates depletion both in interstitial carbon and in substitutional Al, implying the probable presence of C vacancies as well as Al vacancies or antisites on the Al-sublattice.

To understand the experimentally determined off-stoichiometric κ-carbide compositions, DFT calculations are performed which determine the

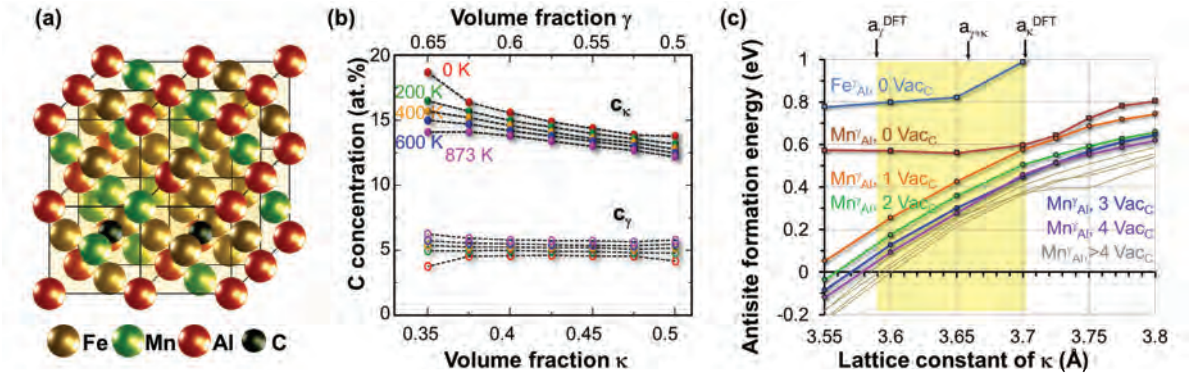

Fig. 2: *(a) 2x2x2 supercell adopted in DFT calculations with the κ-precipitate composition measured by APT - $Fe_{16}Mn_6Al_7C_5$ ($Fe_{2.0}Mn_{1.125}Al_{0.875}C_{0.625}$). (b) Carbon concentrations in κ-carbides and the γ-matrix as a function of their volume fraction at different temperatures including the experimental annealing temperature of 600°C (873K). (c) Mn antisite formation energy as a function of the lattice constant for different numbers of carbon vacancies.*

energetic stability of these different possible defects. Thermodynamic concepts were developed and applied to fully consider the experimental constraints in terms of local composition (Fig.2a). Importantly, there is a remarkable effect of volumetric strain on C vacancy formation energy – the more the κ-carbides are compressed, the more the C vacancies are energetically favored. Thus, the measured depletion of C in κ-carbides is a consequence of compressive coherency stresses exerted by the γ-matrix. As a consequence, we predict a decrease of the C content in κ-carbide with the κ/γ volume fraction, since this ratio determines the elastic misfit energy (Fig.2b). Due to configurational entropy the driving force on C to leave κ-carbide becomes even stronger at finite temperatures, as can be seen in particular for the experimental annealing temperature of 600˚C (873K) in Fig.2b.

However, the sole effect of elastic strain cannot explain the Al off-stoichiometry since the vacancy formation at an Al site is energetically unfavored even under volumetric compression. Further, the Al depletion caused by the formation of Mn^{γ}_{Al} antisites (Mn atoms from the γ matrix replace Al atoms in κ) in an otherwise perfect κ phase arising from this effect is three orders of magnitude lower than the experimentally measured one. However, when combining the effects of strain and C vacancies within DFT calculations a drastic effect on the stabilization of Mn^{γ}_{Al} antisites is observed that is in the right order of magnitude to explain the experimental values (Fig.2c). The preference for the formation of Mn^{γ}_{Al} antisite in the vicinity of C vacancies can be explained by the strong binding energy between Al and C under volumetric constraint. It gives rise to a high retention of Al to the κ-carbide, but the reduction of the carbon concentration makes the presence of Al in the κ-carbide less favored.

Based on the combination of APT and DFT investigations – i.e. the joint effort of two departments – it was, thus, possible to understand the off-stoichiometric composition and corresponding elemental site-occupancy of κ-carbides in an austenitic Fe-Mn-Al-C steel: In such a κ/γ system with coherent κ-carbides embedded in γ-matrix, the alloy tends to minimize the elastic strain energy and stabilize the two-phase microstructure by having C vacancies and Mn^{γ}_{Al} antisites (Fig.2a).

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Coarsening Kinetics of Lamellar Microstructures of Fe-Al *in situ* Composites – Experiments and Simulations

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Fe-Al alloys in the composition range of about 55 to 65 at.% Al undergo a rapid eutectoid phase transition at 1095 °C resulting in an *in situ* composite material with a fine-scaled lamellar microstructure with average lamellar spacing λ of about 200 nm in as-cast material [1] (Fig. 1). During this instantaneous solid-state reaction, the high-temperature phase Fe_5Al_8 with a cubic, γ brass-type structure decomposes into a mixture of the crystallographically closely related phase B2 FeAl and the triclinic phase $FeAl_2$ [2,3]. Very similar fine-scaled lamellar microstructures consisting of two intermetallic phases are well-known from Ti-Al-based alloys, where they lead to a combination of well-balanced properties in terms of creep, ductility and strength.

The coarsening behaviour of the fine microstructures was investigated in dependence on time and temperature by detailed experimental work and compared to results of phase field simulations. On the one hand, the knowledge about the coarsening kinetics is of particular importance to explore the potential of such lamellar FeAl + $FeAl_2$ alloys as candidates for high-temperature applications. On the other hand, the extended, nearly perfect lamellar microstructures offer an excellent possibility to study the kinetics of coarsening of lamellar structures in general and compare the observations to existing theoretical models.

An Fe-Al alloy containing 60.9 at.% Al, which corresponds to a fully-lamellar microstructure, was synthesized by induction melting and pieces were heat-treated at 600, 700, 800, and 1000 °C for various times ranging from 10 min up to 5000 h. Heat treatments were performed in an Ar inert atmosphere and all samples were finally quenched to room

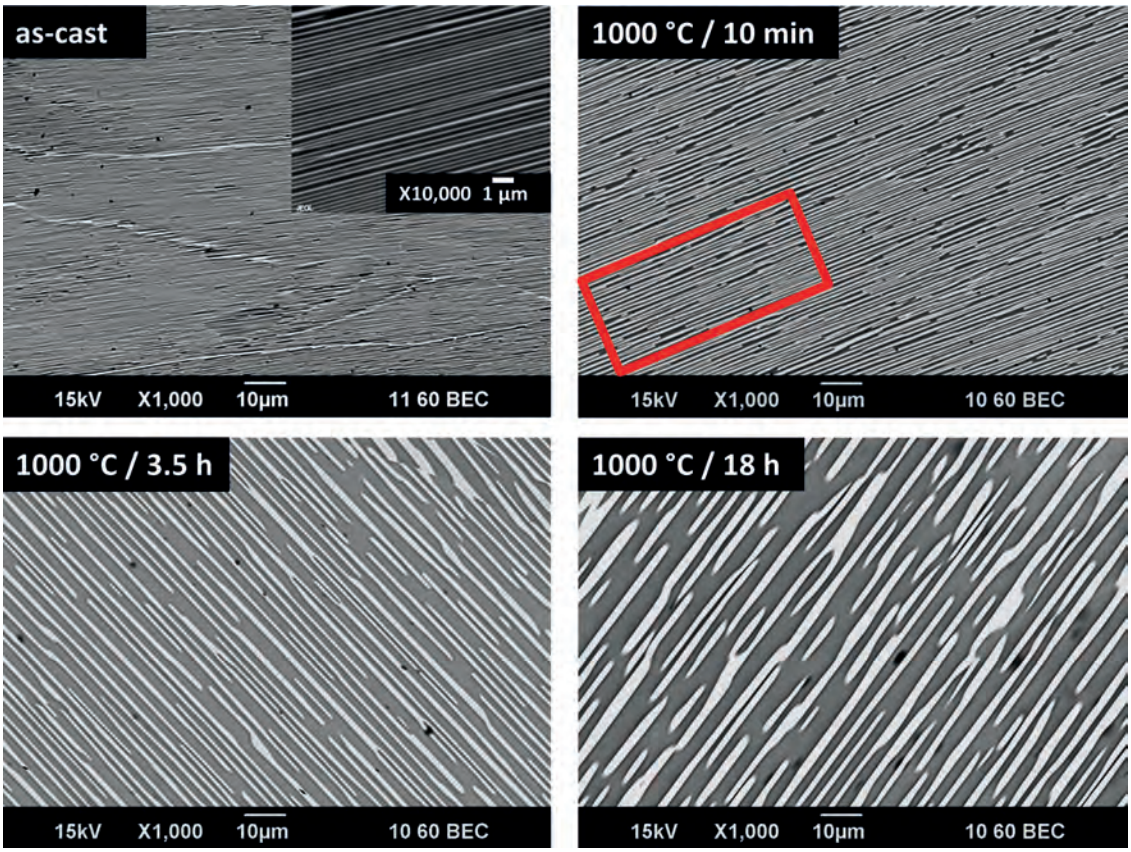

Fig. 1: *Coarsening of the lamellar FeAl + $FeAl_2$ microstructure of an Fe-60.9 at.% Al alloy after different times at 1000 °C (scanning electron microscope pictures obtained in back-scattered electron mode). The red region shows the domain that is used for the phase field simulations as input.*

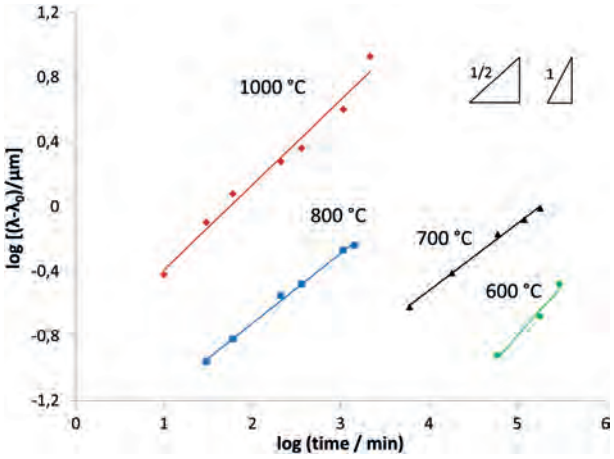

Fig. 2: *Double-logarithmic plot of the increase of the lamellar distance as a function of time.*

temperature. The true lamellar distances were determined by a special procedure taking into account the 3D nature of the microstructure. In a first step, an extended lamellar area on the surface of a sample was oriented with the lamellae extending parallel to the *x* or *y* direction, and in the next step, the surface was vertically cut perpendicular to the lamellae orientation by focused ion beam. To observe the new surface, the sample was tilted and the distance of the lamellae as well as the angle between the lamellae and the edge between original and new surface were measured. From these values and the known tilting angle, the true lamellar distance can be calculated by simple geometrical considerations. In this way, at least ten values were determined per sample. Each data point in Fig. 2, which shows the increase of the lamellar distances as a function of time for different temperatures, corresponds to the average value of such a procedure.

As an example, Fig. 1 shows the development of the microstructure after different heat treatment times at 1000 °C. At this high temperature, coarsening as expected is very quick and after times longer than 36 h, the lamellae have already spheroidized so strongly that it is no longer possible to get a reliable value for the lamellar spacing. At lower temperatures, the coarsening kinetics is very much slower; e.g. after 5000 h holding at 600 °C, the lamellar distances are still smaller than after only 10 min at 1000 °C. As is visible from Fig. 2, the time dependence of the increase of the lamellar distance can be well described by simple power functions with exponents of 0.6(1), 0.41(1), 0.42(1), and 0.51(5) for 600, 700, 800, and 1000 °C, respectively.

Theoretical models for the coarsening of lamellar systems have been developed by Graham and Kraft [4] and Cline [5], which predict different scaling laws for the coarsening. The Graham-Kraft model leads to a scaling of the lamellar spacing according to $\lambda \sim t$, whereas Cline predicts a slower scaling with time t according to $\lambda \sim t^{1/2}$. The present experimental investigations indicate that the Cline model leads to an appropriate description,(Fig. 2).

To further shed light on the different analytical descriptions, we have developed a diffusion-limited alloy phase field model to predict the coarsening kinetics also numerically. The basic ingredient of both above theories [4,5] is the shrinkage kinetics of lamella terminations driven by surface energy minimization. The anticipated scaling of the shrinkage velocity $v \sim 1/\lambda^2$ is verified by the phase field simulations, whereas a Cahn-Hilliard model leads to more sluggish kinetics. This outcome is the basis for two-dimensional phase field simulations with experimental microstructures as initial condition (Fig. 3). The coarsening of the lamellae can clearly be seen, in analogy to the experimental results in Fig. 1.

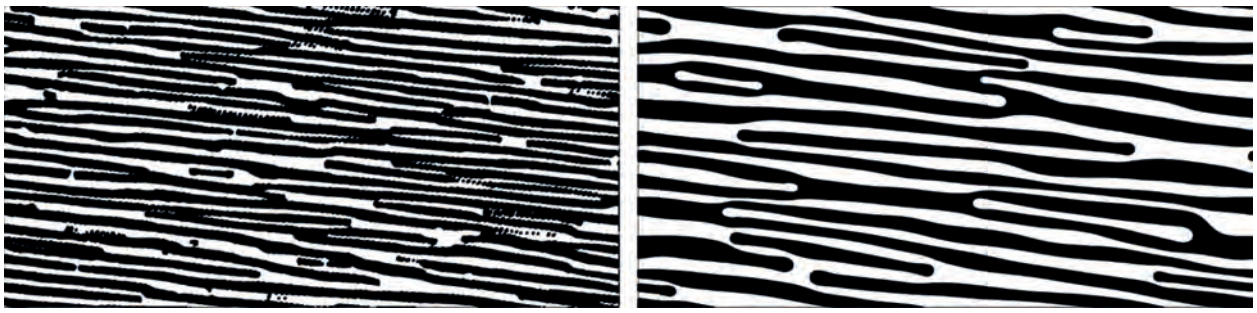

Fig. 3: *Two-dimensional phase field simulation of lamella coarsening, using the red section in Fig. 1 as initial condition (left). The right panel shows a snapshot of the coarsening process.*

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Atomic Structure and Properties of Silicon Grain Boundaries

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Grain boundaries (GBs) in materials have substantial influences on device properties, for instance on mechanical stability or electronic minority carrier lifetime in multicrystalline silicon (mc-Si) solar cells. This applies especially to asymmetric, less ordered or faceted interface portions. Here, we present the complex atomic interface structure of asymmetric and faceted tilt grain boundaries in silicon, observed by high resolution scanning transmission electron microscopy (HR-STEM) and explained by atomistic modeling and computer simulation. As an outlook, newest results of a faceted Σ3 GB analyzed by HR-STEM and atom probe tomography (APT) are presented as well as first results of microscale fracture tests.

Hardware aberration corrected HR-STEM enables us to distinguish individual atomic column positions having projected distances around an Ångstrom or below [1,2]. Contrary to the well-known symmetric Σ9(122) structure in Si, the atomic structure of the observed asymmetric Σ9 (111)|(115) segment shows strong distortions, but nevertheless it repeats periodically with almost perfect accuracy over a range of several 100 nm. At the interface we identify 10 Si dumbbells, which cannot be assigned to one of the two grains, as they have a completely different orientation. Furthermore, there are four apparently single-atomic columns per period. The distorted dumbbells are oriented such that they resemble the structure of several short stacking faults or "nano-Σ3 twin boundaries", consisting of only 4 to 8 atoms.

Starting from the experimental HR-STEM images, a preliminary atomistic model of the asymmetric GB was created by placing Si atoms at the intensity-peak positions. Free surfaces to a vacuum volume were introduced in the structure model to terminate the two grains in the relaxation calculations. The orthorhombic super-cell with periodic boundary conditions contains a slab of 360 Si atoms and extends over 19.95 Å along the interface, over 56.96 Å perpendicular to the interface, and over 7.679 Å along the viewing direction.

Classical atomistic molecular-statics simulations using empirical interatomic potentials, namely Tersoff [3], Stillinger-Weber [4] and EDIP [5] potentials, have been used to relax the interface structure and to calculate the GB energy. The relaxed structure shows qualitatively a good match between experiment and calculation. It turns out that the atoms in the apparently single-atomic columns are three-fold coordinated in the non-relaxed configuration, but can reconstruct to four-fold coordination by pairwise displacements along the [110] direction. Within the used super-cell eight possible reconstruction patterns exist. To study the thermodynamic stability of the GB and its dependence on the various reconstruction patterns of the single atomic columns, GB energies have been calculated. It is known that empirical potentials yield correct GB structures but overestimate interface energies [6-8]. In order to elucidate this deficit, interface energies for a set of different

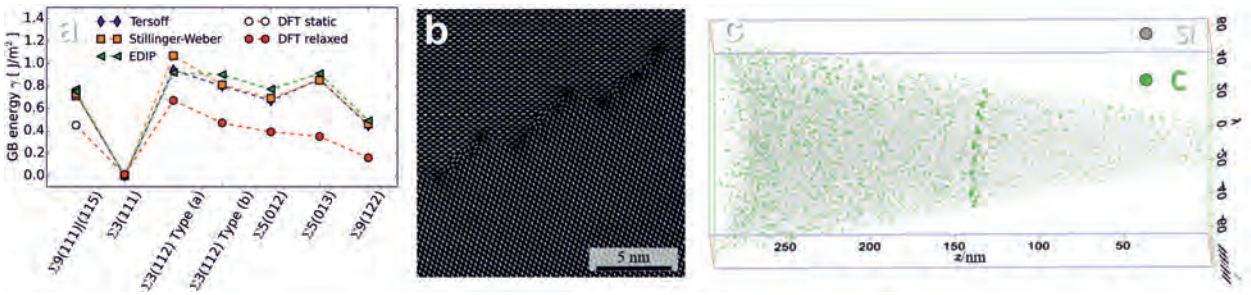

Fig. 1: *(a) Calculated GB energies for various GBs. DFT values are taken from [9]. The DFT value of the GB energy for the asymmetric Σ9(111)|(115) has been obtained from a static calculation using the relaxed structure as obtained by empirical potentials. The Σ3(112) GB types termed as (a) and (b) correspond to the symmetric and asymmetric Σ3(112) GBs, respectively in [9]. (b) Experimental HR-STEM image of faceted Σ3(112) GB. (c) Projection of 3D APT data (LEAP 5000) from the very same GB showing C segregation along lines at the GB position.*

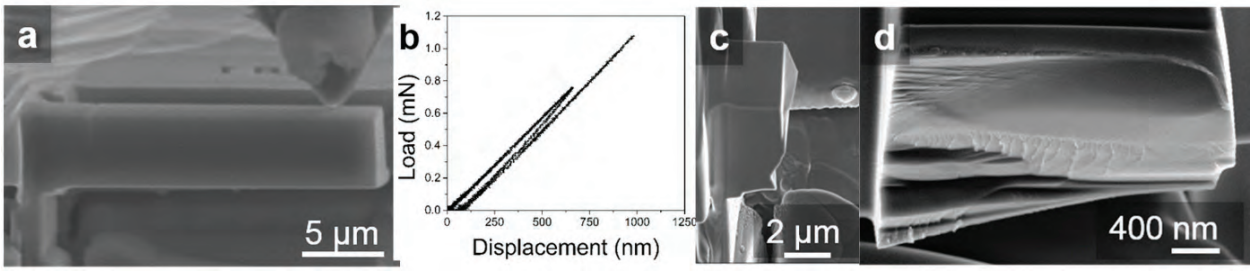

Fig. 2: *Miniaturized bending beam for fracture testing of grain boundaries in Si: (a) in situ SEM image of loading configuration (b) Load - displacement curve (load – unload cycle) obtained from in situ SEM bending, (c) side and (d) front – view images of fractured interface.*

GBs have been calculated and related to *ab-initio* density functional theory (DFT) results which have been previously obtained [9]. The energy of the observed structure is found to be in the range of the highly symmetric low-Σ GBs, Fig. 1(a). This explains its stability over a large spatial region of more than 100 nm. The relaxation of the GB structure into a sequence of short Σ3 nano-TB segments could be one reason for the surprisingly low energy values for this complex GB structure.

For further atomistic simulations and a complete understanding of the GB physics, it would be of highest interest to know the GB chemistry with highest accuracy. To face this problem, we combined the sample preparation of HR-STEM thin foils with the sample preparation of APT tips by focused ion beam (FIB). This enables us now to analyze the structure of a GB by HR-STEM and the chemistry of the same GB by APT. A first result is shown in Fig. 1, where (b) shows the facets of a Σ3(112) GB and (c) shows C segregation along lines at the GB position in the 3D APT data. This suggests a preferential segregation of the C impurities at special GB features. The additional chemical information can be implemented into the simulations in the future and will lead to a more thorough understanding of GBs in general.

Si as a brittle material permits to perform miniaturized fracture experiments as we have recently proved with different small scale fracture experiments all fulfilling linear elastic fracture mechanics [10]. Currently, we try to determine with notched bending beams the interfacial fracture toughness values of the grain boundaries described above, Fig. 2. The values will be compared to the work of separation obtained by DFT calculations and the fracture paths characterized by electron microscopy and AFM studies.

In conclusion we studied the atomic structure of asymmetric and faceted GBs in mc-Si by HR-STEM. In case of the Σ9(111)|(115) interface an energetically favorable substructure is found explaining the surprisingly low GB energy found in the molecular statics calculations. Correlation of HR-STEM and APT data allows access to the exact GB chemistry and will improve the atomistic simulations in the future.

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Integrated Experimental-Numerical Analysis of Stress and Strain Partitioning in Multi-Phase Alloys

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Advanced alloys typically have microstructures composed of multiple phases. Through thermo-mechanical control of the crystallography, composition, morphology and relative fractions of these structural units, a wide property spectrum can be accessed. It is however a challenging task to design optimal microstructures that would satisfy the property combination specifications for a given application. In the case of automotive steels, for example, a coupled increase in both strength and toughness is sought for simultaneous improvements in weight reduction and crashworthiness. Yet, micro-mechanically verified microstructure design guidelines that would allow achieving this goal, are at present not available. To this end, an experimental-numerical methodology has been developed at the MPIE that enables high resolution tracking of deformation induced microstructure, micro-strain and micro-stress fields, through *in-situ* scanning electron microscope (SEM) deformation experiments and accompanying crystal plasticity simulations (Fig. 1) [1].

Both, experiments and simulations, start with electron backscatter diffraction (EBSD). In the former, to allow simultaneous micro-strain and microstructure mapping, a recently developed digital imaging correlation (DIC) technique is employed that provides strain maps without inhibiting microstructure mapping by EBSD, electron channelling contrast imaging (ECCI) and scanning electron (SE) imaging measurements. The simulation route uses the EBSD map to create a crystallographically informed numerical model with phase properties obtained from inverse crystal plasticity finite element method (CPFEM) simulations of nanoindentation experiments. Using a recently developed spectral solver suitable for heterogeneous materials with high mechanical phase contrast and nonlinear stress–strain response, full-field CP simulations are carried out (Fig. 1).

The approach has so far been applied to martensitic steels, bainitic steels and martensitic-ferritic steels [2,3]. As shown in Fig. 2 for the latter, the overall approach provides a unique overview of

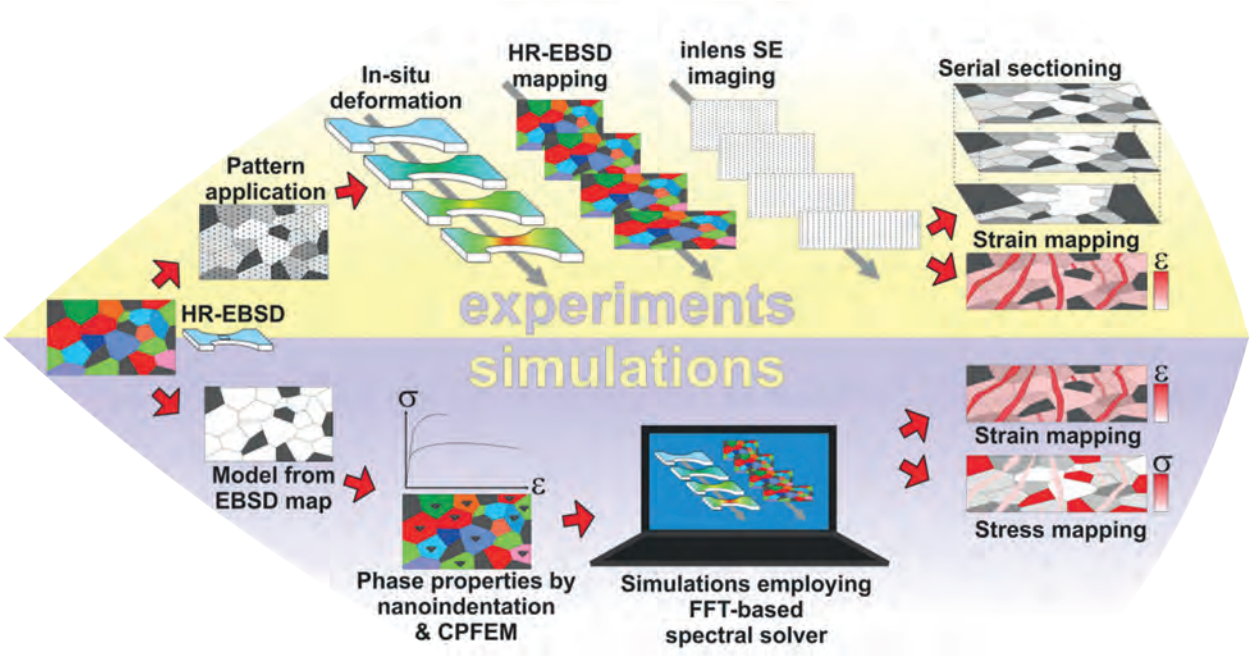

Fig. 1: *The integrated approach involves experiments and simulations both proceeding from the same EBSD-mapped microstructure data set, providing the local strain and stress distribution maps as well as the microstructure changes [1].*

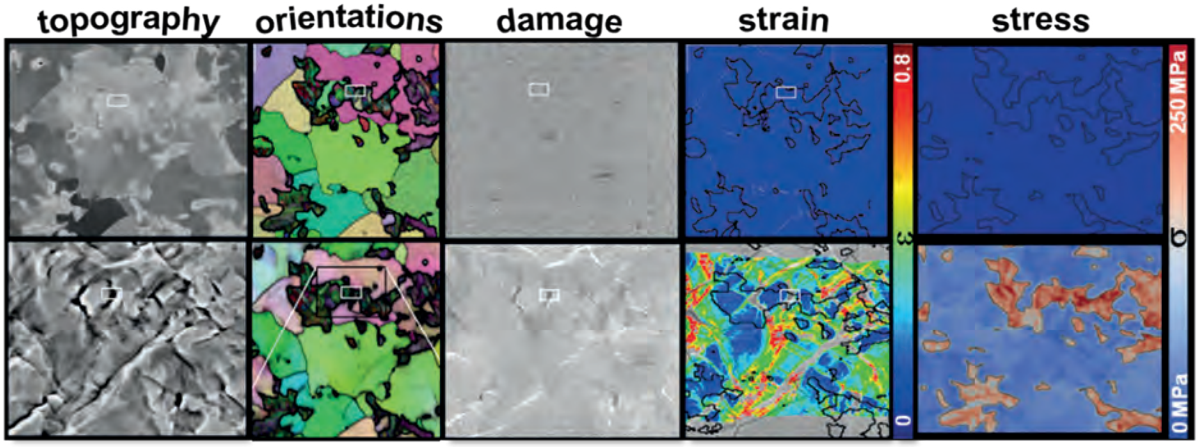

Fig. 2: *The results of dual phase steel: SE imaging reveals topography, EBSD reveals orientation changes, inlens SE images reveal damage incidents, DIC reveals local strains, and CP simulations reveal the local stresses [2, 3].*

all the inter-linked micro-processes taking place during deformation: topography formation, crystallographic rotations, damage nucleation, strain and stress localization, etc. The realm of data produced thus reveals various key insights on how novel alloys can be developed for targeted mechanical response [3].

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Broadband Reflecting Microfibers with Tailored Structures Inspired by Desert Ants

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Over millions of years, living organisms have evolved and optimized complex, three-dimensional structures on length scales suitable to interact with and manipulate solar light, thus achieving effects that are essential for their survival, like signaling, camouflage or warning [1]. Despite consisting of low refractive index materials, they show highly adapted and efficient photonic properties that have attracted the attention of scientists aiming at the design and development of new optical materials [2, 3]. So far, the majority of such studies have concentrated on structures exhibiting periodical order [4, 6]. However, an increasing number of recent studies shows that nature also evolved photonic structures featuring various degrees of disorder [7], which display well defined optical properties that could not be achieved with periodically ordered structures consisting of the same materials.

In terms of adaptation to specific habitats, deserts are particularly challenging for insects due to the extreme variations in temperature and the extreme insolation during day-time. Nevertheless, ants (Insecta, Hymenoptera, Formicidae) like the Saharan silver ant Cataglyphis bombycina (Fig. 1a) have successfully adapted by evolving long legs to keep the body away from the hot sand, visual orientation based on the position of the sun instead of pheromone orientation and the ability to produce sophisticated heat shock proteins that ensure the function of their metabolism at very high body temperatures [8]. The body of these ants is densely covered with setae (Fig. 1a) that give them a metallic silver-like sheen (Fig. 1b). This indicates that the optical properties of the setae are adapted to shield the animals from sunlight through broadband reflection, thus preventing additional heating up. The fact that setae are fibres makes them a very interesting photonic system that is suitable as a biological blueprint for the development of novel synthetic organic fibres with tailored reflective properties.

Structural characterization of the setae shows the elongated, needle like shape of the setae (Fig. 1b) which are uniformly about 80µm long and have a thickness of about 3.5 µm. Their cross section has the shape of an isosceles triangle. Both lateral surfaces of each setae are decorated with a quasi-ordered pattern of longitudinal microribs with a spacing varying between 180 and 220 nm (Fig. 1c). The underside of the setae is flat and unstructured (Fig. 1c, insert). Every setae is pervaded by an irregularly shaped central canal (Fig. 1d). Fractured setae reveal a solid interior consisting of densely packed filaments that appear to be co-oriented with their long axis (Fig. 1e). In the larger bundles of setae observed in densely covered cuticle areas, the setae are randomly stacked and are connected in the contact areas by a soft, waxy material (Fig. 1g). Measurements of the overall reflectance of exoskeleton parts covered with setae using Fourier transform infrared (FTIR) spectroscopy show broadband reflection resulting from homogeneous reflection and scattering of all wavelengths with an efficiency of up to 40% (Fig. 2a). Transmittance spectra of isolated setae placed on glass slides (Fig. 2b) show

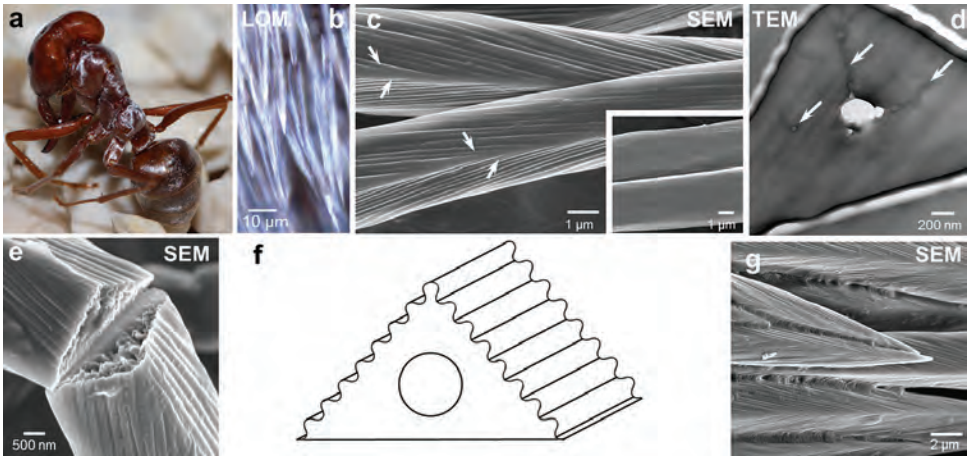

Fig. 1: *(a) Habitus of Cataglyphis bombycina workers. (b) Light micrograph of bundles of setae. (c) Electron micrograph of individual setae showing their triangular shape and the microribs (arrows) covering the side surfaces. The insert shows the smooth unstructured underside of the setae. (d) Transmission electron micrograph showing the central canal. (e) Cross-fractured setae revealing the disordered internal structure. (f) Schematic depiction of the setae architecture. (g) Cluster of setae where the contact areas are fused by a waxy substance.*

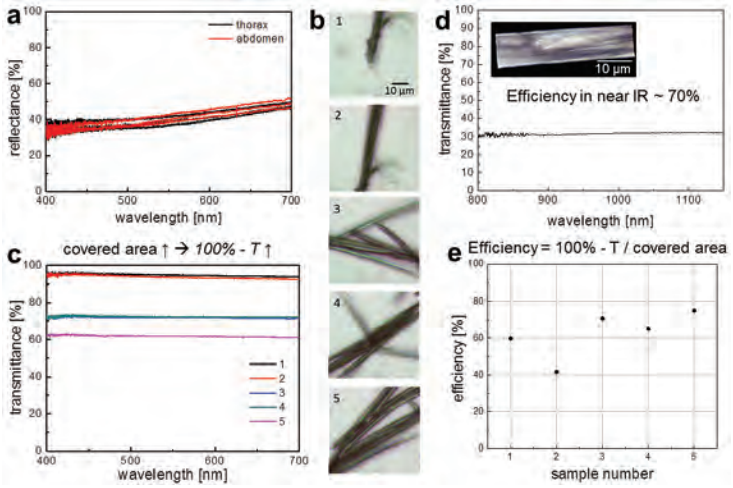

Fig. 2: *(a) Reflectance spectra recorded on different parts of the body of Cataglyphis bombycina. (b) Areas of glass slides covered with setae used for the transmittance experiments. (c) Transmittance spectra recorded for the samples in (b). (d) Transmittance spectrum of setae (insert) in near IR. (e) Shielding efficiency of the setae as ratio covered area / 100% - T.*

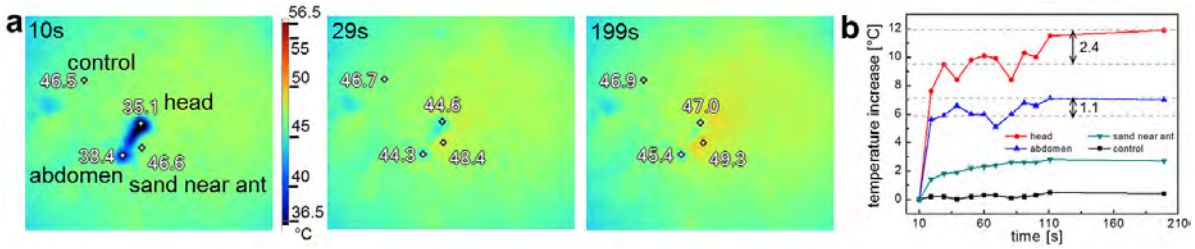

Fig. 3: *(a) Thermographic images recorded at 10s, 29s and 199s after placement of the ant, the numbers are temperature values [°C]. (b) Diagram of the temperature increase with exposure time monitored for head and abdomen of the ant and the sand substrate. The arrows between dashed lines indicate the temperature increase of head and abdomen between 29 s and 199 s exposure time.*

that if the covered area increases, the transmittance decreases (Fig. 2c). The calculated efficiency of shielding light for the setae can be as high as 75% for the visible (Fig. 2e) and 70% for the near infrared (IR) wavelength ranges (Fig. 2d).

This shows that the setae are very efficient in shielding from solar radiation. The thermoregulatory function of the setae is confirmed by thermographic analysis of the ant body in a setup simulating their native environmental conditions (Fig. 3a). The results show that the temperature of the abdomen, which is densely covered with setae, increases slower than the temperature of the head where only few setae are present (Fig. 3b).

The overall goal of this interdisciplinary collaboration between the MPIE and Paderborn University is to establish design rules for artificial organic textile fibers with highly efficient broadband reflection properties that are generated by an irregular architecture and tailored structural disorder on the micro- and nanoscopic length scale. Further structural, compositional and optical characterization combined with a theoretical study of their function will yield complete sets of data that can be used to fabricate polymer-based biomimetic high-reflectivity fibers using techniques like direct laser writing in collaboration with Prof. von Freymann, University of Kaiserslautern and Prof. Zollfrank, Technische Universität München.

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Magnetism at the Domain Walls of an Epitaxial Oxide Thin Film

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The coupling between magnetic and ferroelectric order parameters in magnetoelectric multiferroics has drawn considerable research interest due to their potential application as multifunctional devices [1]. Among perovskite manganite based multiferroics, orthorhombic $TbMnO_3$ (TMO) is a prominent candidate because of its large magnetoelectric coupling and since its ferroelectric state is directly coupled to the magnetic structure. In bulk orthorhombic TMO below 28 K, the magnetic interactions between nearest neighbours and next-nearest neighbours stabilize a cycloidal spin structure of the Mn sublattice. The magnetic cycloid breaks inversion symmetry and induces a macroscopic electrical polarization (via the inverse Dzyaloshinskii-Moriya interaction). Thus, TMO is a multiferroic material with a strong magnetoelectric coupling. Additionally, TMO exhibits a sinusoidal antiferromagnetic state which exists between 28 K and the Neel temperature at 42 K [2,3].

Epitaxially stabilized thin films offer the possibility of utilizing the misfit strain to have additional degrees of freedom for tuning the properties that are different from the bulk. The misfit strain allows the system to have different symmetries and nanometer sized regions that exhibit new functionality, e.g. epitaxial TMO films grown on $SrTiO_3$ (STO) substrates exhibit net magnetic moments. The proposed origin for the

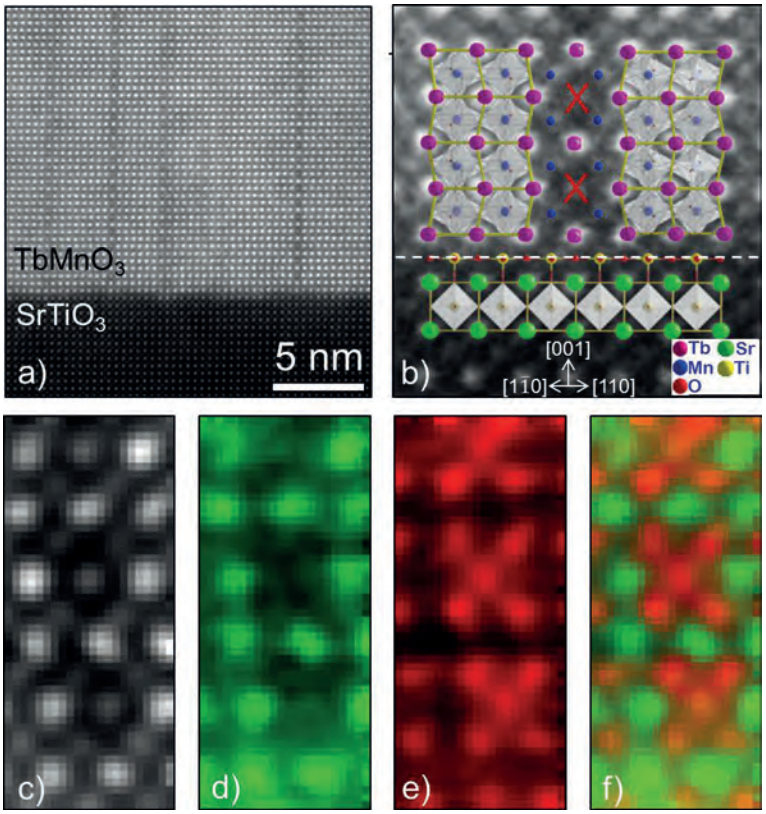

Fig. 1: *a) Atomic resolution HAADF-STEM image showing the interface of $TbMnO_3$ on $SrTiO_3$ substrate. Domain walls are seen as a vertical line in the $TbMnO_3$ thin film. b) Crystallographic structure and orientation relationship is overlaid on the domain wall for better visualization. The position "X" in the image is where the additional Mn atom is detected. c) HAADF signal collected simultaneously during the spectrum image acquisition of the domain wall. d) and e) Integrated intensities of the Tb $M_{4,5}$ and Mn $L_{2,3}$ edges from the spectrum image. f) Overlay image of d) and e) showing the clear presence of an additional Mn atom replacing Tb. Image adapted from [6].*

net magnetic moments in this system has been attributed to epitaxial strain-induced unit cell deformation, leading to the changes in their magnetic interaction. However, the epitaxial strain at the substrate - film interface alone does not reveal the reason behind the observed phenomena [4]. With the help of atomically resolved high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) and electron energy loss spectroscopy (EELS), in addition to the different crystallographic domain [5] we have found a one atomic layer thin domain wall with distinct chemical signature. Investigating this domain wall with a state-of-the-art transmission electron microscope resolved the origin of the ferromagnetic phase in TMO [6]. The high strain concentrated at the domain wall modifies the structure and composition along the domain wall. The domain wall consists of an additional Mn atom in the position of the Tb atom. The canting of the Mn spin is responsible for the observed net magnetic moments. The long range spiral spin ordering along the domain structure is disturbed by the presence of the domain wall. The density of the domain wall can be tuned upon the thickness allowing up to 25 percent of the total volume. We have also established a relationship between the density of domain wall, film thickness and net magnetization in the film. The detailed magnetic studies, density functional theory and embedded cluster calculation performed by our collaborators explain the contribution of the domain wall towards the net magnetization observed in these films. Further, we also believe that this kind of novel structures that are normally absence in bulk can be synthesized in thin films by making use of epitaxial misfit strains. This new class of thin 2-dimensional sheets with unique functional properties opens the door for novel applications in nanoelectronics [6].

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Interplay between Defects and Reactive Surfaces

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An accurate description of solid/liquid interfaces and the elementary processes occurring on them is a prerequisite to understanding their reactivity, which is the key to most electro-chemical and colloidal processes of practical importance. It encompasses (but is not limited to) knowledge about interface structures, their stability, growth and evolvement, which directly couples to defects and their impact, e.g., on reactions.

One illustrative example is the formation of oxide films on metal surfaces, which can dramatically increase the corrosion resistance of materials and are of utmost importance when we consider the tremendously important role metals play in our society. A key quantity to understand the growth/dissolution of protective oxide films is the knowledge which defects are present in the oxide in appreciable concentrations and a given electrochemical environment. Utilising the vast knowledge about charged point defects in semiconductors [1] and our recently developed approach that unifies concepts in semiconductor physics and electrochemistry [2] we gained surprising new insights into the Zn/ZnO/H_2O system [3].

Extending the concept of Pourbaix diagrams, which show the most stable bulk and defect (ions in water and other solvents) phases as a function of pH and overpotential, we proposed a scheme to construct defect phase diagrams which span the relevant range of configurational space as defined by the accessible potentials for the chemical species and the electrons [3]. These new diagrams (Fig.1) yield the dominant defect for any thermodynamically allowed combination of oxygen chemical potential and overpotential, and, being formally equivalent to a Pourbaix diagram, are also easily combined with the well-established electrochemical stability region of water (region between the two dashed black lines in Fig.1). The application of the approach to the seemingly extremely well studied oxide ZnO revealed a number of surprises, the most striking result being that charge neutral defects become dominant under electrochemically relevant conditions. Because such defects behave qualitatively different compared to charged ones, such an observation directly impacts strategies aiming to enhance corrosion resistance, by making a passivation layer more intrinsic.

The proposed efficient and physically transparent way of identifying the relevant defects in a passivation layer under realistic electrochemical conditions can help to develop systematic approaches to search for alloys with improved corrosion resistance. In order to model an interface in detail, however, it is necessary to take into account that defects right at the interface may exhibit modified or even unique properties. Even though the actual structure of the interface is often not known well experimentally, *ab initio* simulations of idealized surface and interface structures help to identify the key features of real interfaces. An important aspect is the electric behaviour of the interface. For instance, the appearance of interface states in the band gap of a semiconductor or insulator will pin the Fermi level at the interface to this state. Electrically active interface defects may play a similar role.

Ab initio calculations can identify the atomistic origin of such defect states by investigating candidate structures in different charge states. The interface is

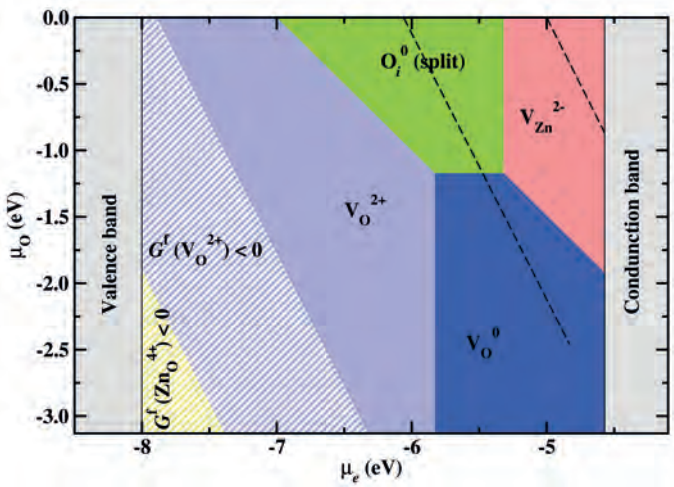

Fig. 1: *Defect stability phase diagram for the Zn/ZnO/H_2O system visualizing dominant defects and conditions for which water is electrochemically stable (region between the dashed black lines).*

typically modelled as a supercell containing several layers on both sides of the interface, and assuming periodic boundary conditions in all three dimensions. Such ordered structures do not directly yield the energetics of randomly distributed, independent defects of interest, notably in charged states where long-range Coulomb potentials and the necessity to introduce a compensating background result in significant variations between different supercells. To correct for these "artefacts", we recently developed a correction scheme along the lines of the sxdefectalign correction scheme for bulk defects [4]. Solving the Poisson equation for the isolated and periodic case with a spatially varying dielectric constant makes it possible to extrapolate the energies of the isolated case already from rather small systems (Fig. 2).

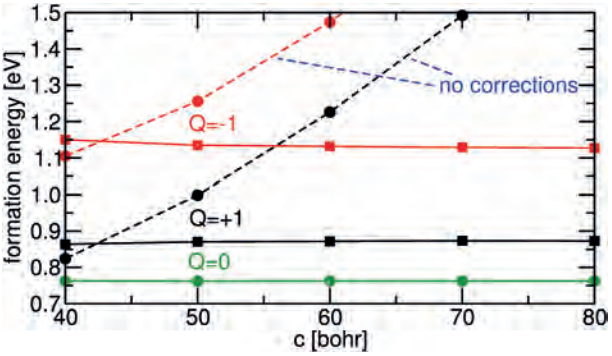

Fig. 2: *Improved convergence of the defect properties with supercell size for a dangling-bond defect at the H-covered Si(111) surface for different vacuum thicknesses and a 2x2 surface cell. Dashed lines connect values as obtained from density functional theory (DFT) calculations, solid lines include electrostatic corrections.*

An example for an application, in which interfacial defects are particularly important are nanoparticles (NPs) embedded in a host matrix, in the context of light emission and solar energy conversion. The resulting electronic and optical properties of such composites are mainly dominated by interfaces. However, very little is known structurally about these composites. In experiment, probing such nano-interfaces with atomic resolution, especially buried ones between the NPs and the surrounding matrix, is extremely challenging.

In the independent NanoMatFutur group „Semiconducting nanocomposites with tailored optical and electronic properties", funded by the German Federal Ministry for Education and Research (BMBF), we investigated NPs with core structures made from exotic Si and Ge allotropes. These are of particular interest with respect to multi-exciton generation (MEG), where one incoming photon creates multiple electron-hole pairs. Calculating MEG rates from first principles, we demonstrated the metastable BC8 phase of Si to feature band gaps that are much more suitable for solar energy conversion and significantly higher MEG rates compared to diamond-like Si NPs [5]. BC8 NPs can now be synthesized and stabilized kinetically in colloidal solutions. Employing massively parallel *ab initio* molecular dynamics we prepared models of matrix embedded Si NPs (cf. Fig. 3). Our calculations predict that low defect densities and favourable band alignments at the NP-matrix interface, obtained from many body perturbation theory, can indeed be achieved [6].

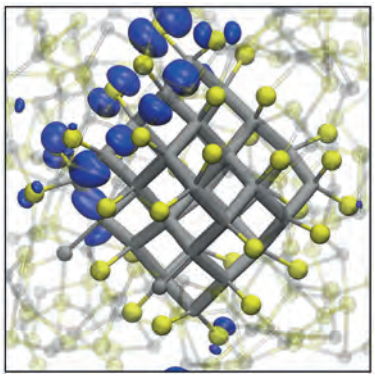

Fig. 3: *Si_{35} NP with sulfur shell embedded in a-ZnS. The HOMO state, illustrated by blue iso surfaces, is localized to the sulfur shell [6].*

To interpret experiments and model the NP-matrix interface in detail, we investigate the various NP surface orientations present at the interface by *ab initio* thermodynamics. The employed wet chemical synthesis techniques require taking the solid-liquid interface at the NP surface and the presence of charged species into account. In particular defects in different charge states are expected to have a strong impact on the composites' electronic and optical properties.

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Hydrogen Detection in Ni-Nb Model Alloy

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Due to its excellent corrosion resistance, the Ni-based Alloy 718 is often used in applications, where it is exposed to hydrogen, such as sour gas environments in oilfields. Since the danger of hydrogen embrittlement (HE) under these conditions seems to correlate with the mechanical properties, the accepted strength classes in the applications are limited. Our research supports the hypothesis that it is the microstructure that determines the sensitivity to HE. In particular, it has been shown [1] that the δ-Ni_3Nb phase plays a significant role in altering HE sensitivity of alloy 718. Furthermore, H-induced vacancies have recently been reported to support HE. With our experimental and theoretical investigations we achieve a better understanding of the real mechanisms behind these assumptions.

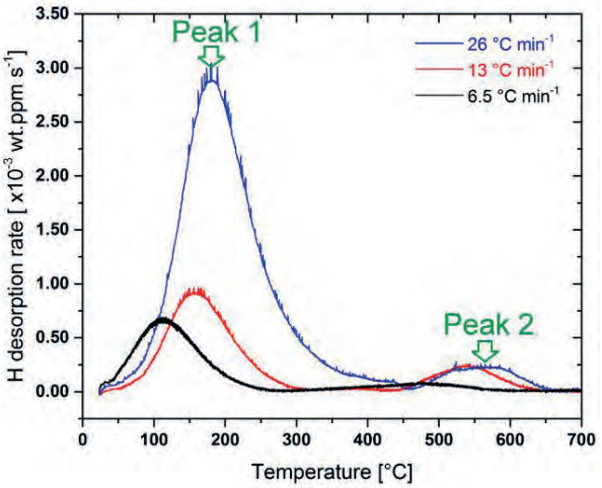

Fig. 1: *Hydrogen thermal desorption spectra of Ni-22wt.-%Nb alloy at different heating rates.*

Major achievements have been made in identifying the hydrogen trapping states and visualizing the hydrogen distribution in the microstructure, which are of primary importance for a concurrent discussion of the H-assisted failure mechanism. Our novel approach correlates measurements using Thermal Desorption Spectroscopy (TDS), Ag decoration technique [2], Scanning Kelvin Probe Force Microscopy (SKPFM) with Pd detection layer [3], and Secondary Ion mass Spectrometry (SIMS). A binary Ni-22wt%Nb model alloy was used to narrow down the parameters of the complicated microstructure in alloy 718 and to elucidate the H distribution and desorption behaviour of the δ-Ni_3Nb intermetallic phase with respect to the γ-matrix.

The relevance of the δ-Ni_3Nb phase was first identified by TDS measurements, where H desorption peak (peak 2) corresponding to an activation energy of 51 kJ mol^{-1} was detected in addition to the typical peak for the γ-matrix (peak 1, 22 kJ mol^{-1}).

The picture looks differently, if locally resolved methods to detect diffusible hydrogen are used: The Ag decoration technique, for example, which uses the special activity of atomic H on a metal surface to reduce Ag ions into elemental Ag, revealed no noticeable desorption of diffusible H from the δ-Ni_3Nb phase (Fig. 2). This result was also confirmed by SIMS, a highly sensitive surface technique. Measuring the deuterium distribution in the model alloy, a higher content in the γ-matrix, correlated with higher H solubility was observed (Fig. 3). Finally, even the more sophisticated SKPFM measurements (Fig. 4), which use a Pd detection layer to resolve the kinetics of H desorption behaviour from the microstructural constituents with high spatial resolution, show a dominating release of H from the γ-matrix until around 100 h.

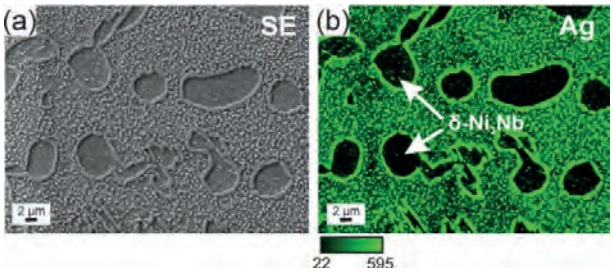

Fig. 2: *Specimen charged with H: (a) SE image of the Ag decorated surface, showing silver particle precipitation on the γ-matrix, indicating the hydrogen flux, (b) Ag EDX map.*

These results are consistent with our *ab initio* calculations, which resulted in a solution enthalpy for H that is 0.5 meV (=50 kJ/mol) higher in the δ-Ni_3Nb phase than in the γ-matrix. The desorption activation energies that were identified by TDS for δ-Ni_3Nb can therefore not correspond to the perfect precipitate phase. According to our calculations, vacancies in the δ phase form one candidate for a deeper trapping site for hydrogen, resulting in a slower release

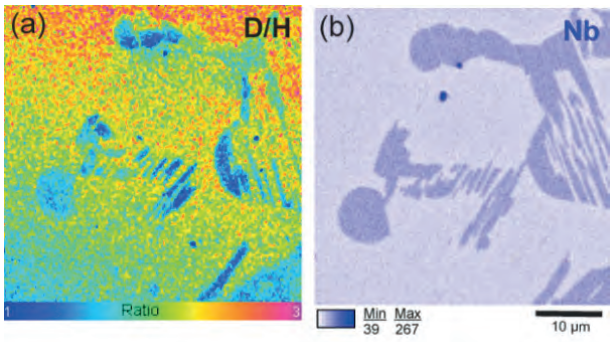

Fig. 3: *(a) Secondary ion map ($^2D^-/^1H^-$). The field of view is 40 µm. (b) Nb EDX map of the scanned area, showing the δ-Ni_3Nb phase as Nb-rich areas.*

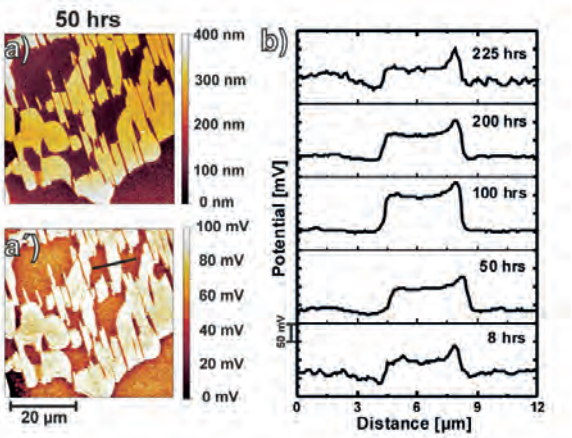

Fig. 4: *SKPFM data obtained for Ni-22wt%Nb: (a) Topography map 50 h after H charging, dark region with lower topography represents the γ-matrix, (a´) potential change on the surface after 50 h, (b) line profiles of surface potential along the black line shown in (a´) over time. Lower potentials correspond to higher H activity.*

in the SKPFM measurements. The increase of their concentration due to the interaction with multiple H atoms has been investigated in the precipitate as well as the γ-matrix phase [4], in order to understand a H-enhanced strain-induced vacancy (HESIV) formation. We reveal that gradients in the chemical potential can provide a driving mechanism for the combination of these vacancies and the formation of nanovoids as recently observed by BSE imaging and further analysed by interrupted tensile testing.

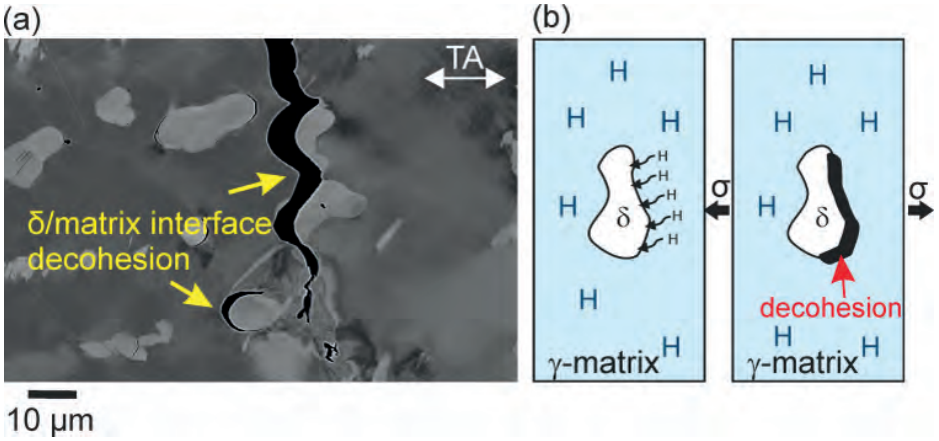

Fig. 5: *Deformation microstructure with H pre-charging: (a) BSE image showing the crack propagation along the δ/matrix interface (TA: tensile axis). (b) Schematic demonstrating the H accumulation and consequent decohesion at δ/matrix interface under an applied stress* σ.

The interface between δ-Ni_3Nb phase and the γ-matrix provides another region of significantly increased trapping and activation energies and is therefore subject to ongoing experimental and theoretical investigations. The accumulation of H at the δ/matrix interfaces under applied loads can lead to the reduction of bonding strength and concurrent decohesion on straining, giving rise to the H-enhanced decohesion (HEDE) mechanism. Indeed, our mechanical testing revealed that such a δ/matrix interface decohesion takes place in the investigated Ni-alloys (Fig. 5a).

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Insight into the Growth of Iron Sulfide Layers in Saturated H_2S Saline Solutions

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Corrosion of iron in H_2S containing solutions is a common problem in oil production and is generally referred to as sour corrosion. Aqueous H_2S solutions promote corrosion of steels, but the exact nature and mechanisms of corrosion strongly depend on the reaction conditions. While the process has been widely investigated for pure iron and carbon steels, there is still a lack of understanding of the reaction path and electronic structure of the corrosion products [1].

For a systematic investigation of corrosion mechanisms, metal was polarized above the corrosion potential in a H_2S-saturated electrolyte to enhance the anodic reactions [2]. Anodic polarisation on iron in de-aerated H_2S saturated acetic saline solutions leads to the growth of an oxide-rich corrosion product with the tetragonal FeS modification mackinawite as the only crystalline component. The mackinawite grows in the (001) direction perpendicular to the base material surface (Fig. 1).

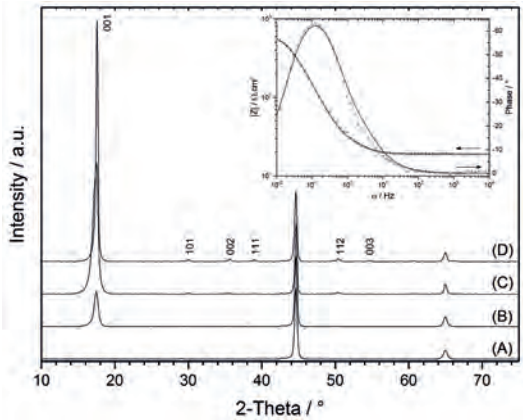

Fig. 1: *XRD pattern of the product scale obtained by anodic polarization of iron for (A) 0 min, (B) 30 min, (C) 120 min, and (D) 240 min. The corrosion product contains the mineral mackinawite without any further detectable crystalline impurities. The reflections at 44.5° and 65° arise from the iron base material. Inset: Bode plot derived from EIS measurement for an iron sample after anodic polarization experiment.*

Optical transmission measurements in the mid and far infrared (IR) have been used to obtain more detailed information about the electronic structure of the electrochemically synthesized FeS. The high absorbance without visible features from vibrational modes throughout the investigated spectral range (4000 - 50 cm-1; 495.9 – 6.2 meV) is characteristic for a strong absorption from electronic transitions. The investigated corrosion products hence do not possess a band gap above the thermal energy at room temperature and are therefore metallic, semi-metallic, or semiconducting with a very low band gap. This result is in agreement with electrochemical behaviour observed: the anodic branch of the linear polarization experiments does not show formation of a protective layer, and charge-transfer resistance determined by electrochemical impedance spectroscopy (EIS) is low (Fig. 1, inset).

X-ray photoelectron spectroscopy sputter depth profiling was used to analyse corrosion products. The results point to the formation of a duplex layer, with an oxide-rich inner part and an oxide-poor outer layer. The formation of the oxide-rich inner layer close to the iron surface can be explained by a large concentration of Fe_{2+} near the interface during dissolution, and the consequent super-saturation of oxide and sulphide. Analysis of cross sections prepared by ion milling indicates that adhesion between the inner oxide-rich and outer oxide-poor layer is poor. Diffraction shows that the distance between mackinawite layers is slightly lower for mackinawite formed during the later stages of the polarization experiments, suggesting that this difference contributes to strain leading to deadhesion. Such a result extends the previous interpretation stating that adhesion between the inner mackinawite layer and outer parts consisting of other sulfide phases is poor. As x-ray diffraction (XRD) shows no crystalline oxide-containing compound (Fig. 1), amorphous fractions, or strongly disordered regions, must be present in the corrosion products.

Amorphous regions are expected to contribute to Raman spectra, however, due to the lack of availability of a normal mode analysis for mackinawite, the interpretation of the recorded spectra is still challenging. More detailed investigations using Raman spectroscopy showed the sensitivity of the formed corrosion products. A transformation of the sulfide compounds (mackinawite) to oxide phases (hematite) has been observed when conducting the experiments ex situ. To avoid the contact of the sample with air oxygen and monitor the corrosion products in their state of formation, *in situ* experiments were executed. The resulted Raman spectra contain only two strong lines at 286 cm^{-1} and 202 cm^{-1}, indicating the formation of mackinawite [3, 4].

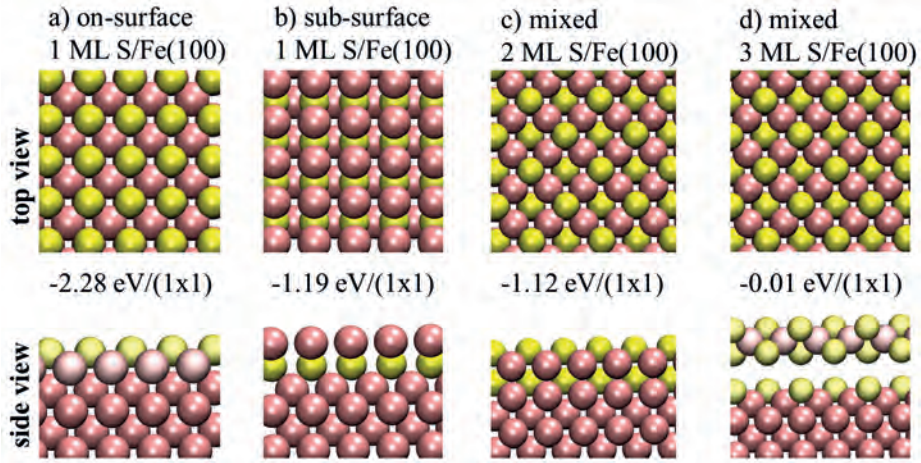

Fig. 2: *Adhesion of low coverage S adsorption phases on the Fe(100) surface. (a) on-surface adsorption of 1 ML S, (b) sub-surface adsorption of 1 ML S, (c) mixed adsorption geometry at 2 ML S forming a S/Fe/S tri-layer, (d) mixed adsorption geometry at 3 ML S, reminiscent of the S/Fe/S stacking in the (100) direction of mackinawite. S=yellow spheres, Fe=red spheres.*

Accompanying theoretical studies focused on the initial states of Fe sulfidation by investigating the adsorption behaviour of S, O and H on the Fe(100) surface by means of density functional theory calculations. These studies revealed for each of the adsorbates a strong preference for adsorption in hollow surface sties. During the ensuing competition H is pushed below the surface, as a consequence of the stronger binding of O and S to Fe. This observation is of interest in the context of H-embrittlement, as it suggests a possible reason for the H presence in Fe bulk. Since hydrogen presents no hindrance to the adsorption of S on the Fe(100) surface, increasing amounts of S attach to Fe in the vicinity of the surface. At 2 ML (at 1 ML, monolayer, the number of adsorbate atoms equals the number of substrate atoms in a layer) sulphur enters the sub-surface region forming a S/Fe/S tri-layer structure, reminiscent of the S/Fe/S planes forming along the (100) direction of mackinawite. This tri-layer adheres strongly to the Fe-substrate [-1.12 eV/(1×1) cell, Area(1×1) = 8.08 Å^2], but adding only one further layer of S significantly reduces the tri-layer's adhesion strength to the substrate. The calculated -0.01 eV/(1×1) cell for the S/Fe/S tri-layer adhesion within the severely laterally strained mackinawite [oriented in the (100) direction] forming on the surface, suggest that flakes of the newly formed corrosion product would easily fall, thus not forming a protective layer and exposing the Fe surface to further corrosion. Poor adhesion is observed experimentally – the FeS indeed does not adhere to the base materials surface well. This lack of adhesion may open the possibility for the formation of oxide-rich corrosion products.

Experimentally, oxide-containing corrosion products were also found under conditions of free corrosion. In contrast to the formation of frequently insulating oxides, a metallic corrosion product does not slow down electron transfer reactions essentially, hence does not protect the base material in the same fashion as an insulating corrosion product. Thorough understanding of corrosion processes in H_2S-containing media hence requires the analysis of the electrochemical properties of the mackinawite-containing corrosion product. An interesting perspective is the investigation of the corrosion of iron-based alloys, where suitable alloy elements may or may not lead to protecting corrosion products.

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From Microbially Induced Corrosion to Bioelectrical Energy Conversion

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Everyone knows rust on iron surfaces, caused by the reaction of atmospheric oxygen with iron that greatly reduces the service life of industrial material. Since rust is oxygen dependent, corrosion of iron would in principle be prevented by the absence of atmospheric oxygen. However, serious cases of damage to pipeline systems in the oil and gas industry frequently show up in oxygen-free soils and marine sediments, with devastating economic and ecological consequences. Hence, corrosion of iron infrastructure in anoxic environments commonly is ascribed to the metabolic activity of microorganisms, primarily sulfate-reducing bacteria and methanogenic archaea that influence electrochemical processes on the metallic surface, causing comparatively high corrosion rates of up to 0.7 mm per year [5, 6]. The

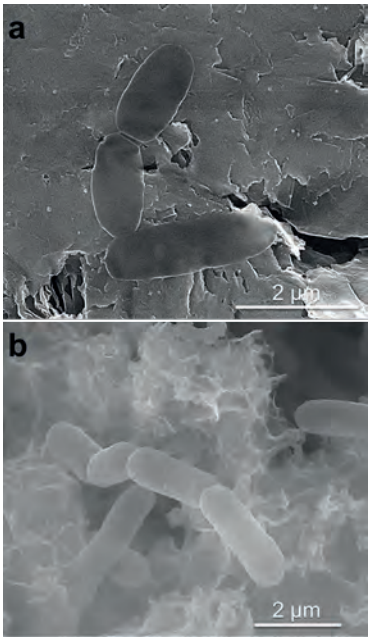

Fig. 1: *Environmental scanning electron micrographs of single cells of Desulfopila corrodens strain IS4. The advantage of graphite cathodes for electrochemical analysis can be seen in the comparison between cells of D. corrodens strain IS4 (a) directly attached to the surface of a graphite cathode and (b) cells attached to a sulfidic corrosion layer on top of an iron specimen.*

decomposition of iron by microorganisms is a major problem, much larger than one might think at first.

In a manner similar to atmospheric oxygen the corrosive microorganisms attack the iron, by using the energy contained in the iron as an energy source for their metabolism, leading to considerable damage of iron infrastructure [6, 7]. However, the basic mechanism by which the microorganisms consume the iron is not fully elucidated. Therefore, electron transfer processes at the electrode/microorganism interface of specialized sulfate-reducing bacteria and methanogenic archaea that are able to take up electrons directly from elemental iron, were characterized in a recent study [2]. In order to provide clear insights into electron transfer processes, electrochemical analysis of the highly corrosive microorganisms was performed in modified bioreactors with a three electrode setup operated with artificial seawater under anoxic conditions and complemented by chemical analysis and scanning electron microscopy (SEM) observations. Especially, direct coupling of precise electrochemical measurements in microbial cultures with chemical analysis like gas chromatography, clearly demonstrated the conversion of electrical energy into microbial end products within the modified bioreactor

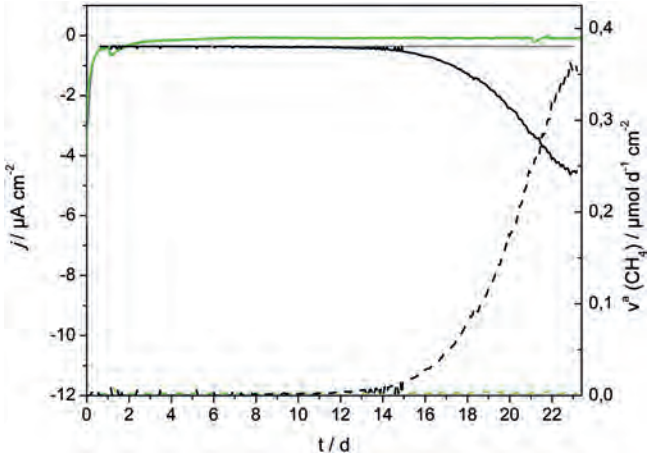

Fig. 2a: *Coupled potentiostatic measurements comparing current densities (solid line) and methane production rates (dashed line) in a sterile control (grey), a control culture (green) and a culture of strain IM1 (black), showing an efficiency of the bio-electrocatalytic process of nearly 80%.*

setup. Moreover, electrochemical monitoring of corrosion rates under those anoxic laboratory conditions for the first time proved that the rather novel electrochemical frequency modulation (EFM) method has a great potential for monitoring microbial corrosion due to the identification of localized corrosion, thereby assessing the accurateness of the obtained corrosion rates [1]. However, the extraordinary electron uptake mechanism of Desulfopila corrodens strain IS4 and the Methanobacterium-like archaeon strain IM_1 at the electrode/microorganism interface is not limited solely to taking up energy from iron surfaces, serving as the sole electron donor for microbial metabolism. Remarkably, the specialized microorganisms also grew on other conductive materials, such as graphite and germanium crystals, when exposed to appropri-

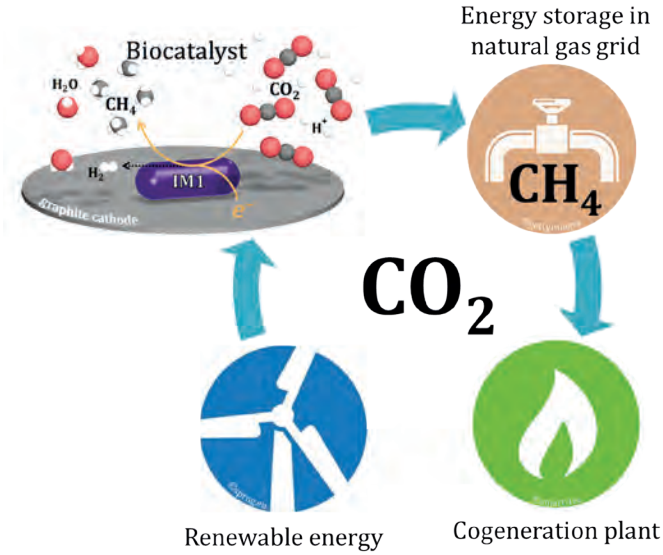

Fig. 2b: *Illustration of bioelectrical energy conversion of renewable energy. A lithoautotrophic archaeon selectively reduces carbon dioxide to methane on a graphite cathode, which can be stored in natural gas grids and reused in cogeneration plants on demand.*

ate power [3, 4]. Those materials for the first time enabled precise electrochemical and infrared spectroelectrochemical analysis of the electron transfer in pure cultures of corrosive microorganisms. Direct electron transfer in the absence of artificial electron mediators was achieved at a potential of -0.4 V vs. SHE. While for strain IM1 the redox active components associated with the outer cell surface are yet unknown, outer membrane c type cytochromes were identified to be involved in a direct electron uptake from reduced surfaces in strain IS4. Thus, strategies can be developed to inhibit the direct entry of electrons into the energy cycle of the microorganisms, preventing e.g. leakage of pipelines.

Moreover, electron uptake from electrodes by specialized microorganisms also is of great importance for an energy conversion process, in which the microorganisms, acting as so-called biocatalysts, convert electrical energy into chemical energy that either can be stored or used as a precursor in chemical production. The great advantage of biocatalysts is the high efficiency in energy conversion and an extraordinary selectivity for distinct conversion reactions, which often is not achieved by conventional catalysts. Coupled electrochemical measurements, especially in cultures of strain IM1, perfectly illustrated its production of methane by the reduction of carbon dioxide, which reached a coulombic efficiency of nearly 80 % at much lower voltages than observed with standard copper catalysts used in the chemical industry [3]. In addition, no other gaseous by-products are produced by those methanogenic archaea, whereby a complicated purification of the emitted biogas becomes unnecessary. Thus, an excess of renewable energy could efficiently be converted at peak times of electricity production into methane through bio electrocatalysis and be stored in an already existing natural gas network without the need of additional storage technologies. In a cogeneration plant the stored energy in the form of methane can thus be used on demand and thereby provides a first solution to the problem of fluctuating electricity production, using renewable energy technologies.

It is noteworthy that investigations of electron transfer processes at the electrode/microorganism interface thus have shown to be not only relevant for elucidating the destructive mechanism of microbial corrosion, but have also shown that this particular mechanism can be exploited for an efficient bioelectrical energy conversion, which is an impressive example of the complexity of bacterial activity and the diversity of bioelectrochemistry.

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Fracture Mechanics and Mechanisms at Small Length Scales

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Micro-scale fracture testing has become an indispensable tool to track the fracture responses of miniaturized materials and devices as well as internal microstructure components with high local resolution [1]. In addition to individual phases in materials, grain boundaries and interfaces between dissimilar materials are in our research focus for downscaling and developing fracture methods with the aim to propose strategies to improve the fracture properties based on sound quantitative fracture data. Our objective is to use site-specific specimen preparation routes like the focused ion beam (FIB) or lithography techniques to machine fracture test specimen and load them using state of the art *in-situ* instrumentation inside the electron microscope to achieve nano-scale load-displacement resolutions and simultaneously visualization of crack propagation. Due to the restrictions imposed by small-specimen sizes vis à vis the microstructural heterogeneity involved, it is hard to find a universal technique applicable for all brittle systems at small-length scales.

The fracture test geometries are either modified versions of bulk fracture test methods or novel techniques [1]. In the absence of ASTM like standards, these are seen to result in a large scatter in KIC as a function of various extrinsic artifacts. In order to quantify the effect of several external factors like loading mode, ion beam damage and notch radius, high purity single crystalline Si without any microstructural complexity was chosen as the model system. We chose four micro-scale test geometries: single cantilever bending, clamped beam bending, double cantilever bending and pillar splitting on FIB-micromachined and FIB-notched specimens on a single wafer of (100) Si and tested them *in-situ* inside the scanning electron microscope (SEM) using a nano-indenter system (Fig 1). The average KIC was measured to be 0.80 MPam$^{1/2}$ with less than 15% variation across the different methods, which is also very close to the macro-scale known fracture toughness of Si [2]. Each test geometry offers certain distinct advantages and limitations [2] and the geometry most optimized for the system concerned is chosen to study the microstructure-fracture property correlation in other systems.

Having confirmed the reliability of the testing method, micro-cantilever bending was used to probe the fracture behaviour of ultra-high strength, heavily cold drawn 0.98 wt % C pearlitic steel wires showing limited ductility and cleavage fracture [3]. These are two-phase lamellar, nanocrystalline nano-composites of α-Fe and θ-Fe_3C used in bridge cables, piano strings and tire cords. Intrinsic length scales of 10-100 nm, and wire diameters of 40 to 150 µm necessitate micro-scale fracture experiments. Fracture tests carried out for drawing strains of 3, 4 and 5 revealed a sharp drop in KIC from 25 to 9 MPam$^{1/2}$ with increasing strain (Fig 2a), with values quite close to macro-scale tests of severely plastically deformed samples [4]. These drawing strains are of interest because they represent a transition regime, where the structure breaks down from a lamellar two-phase material to a nanocrystalline columnar structure of a tetragonal distorted α-Fe with the cementite decomposing and the excess C forced into solid solution of the distorted α-Fe and enriched at the grain boundaries [3]. Preliminary post-mortem analysis of the fracture process shows a mixture of trans-granular and inter-columnar boundary fracture (Fig 2b-c).

A bigger and more practical challenge is to gain insights into adhesion and interface fracture in multilayer thin film systems like those used in protective coatings or microelectronic devices. The role of interface strength within a matrix of brittle

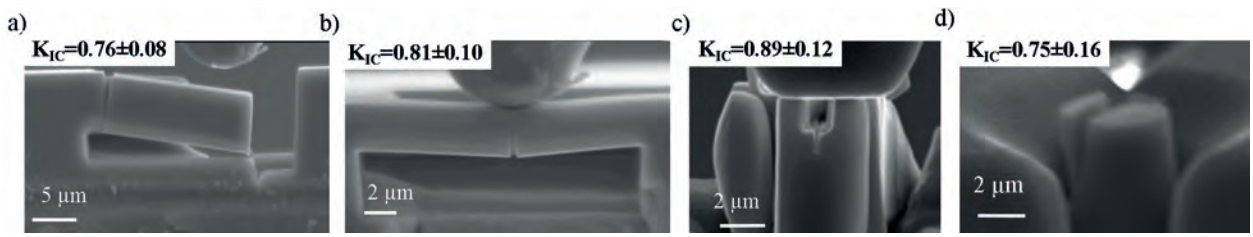

Fig. 1: *a)-d) Four micro-scale fracture geometries tested on Si (100) showing linear elastic deformation till final failure and the corresponding fracture toughness values.*

a)

Drawing strain (ε)	K_{IC} (MPam$^{1/2}$)	Type of fracture
3.2	25.7 (lower limit)	Elastic-plastic, stable
4.2	10.7±1.7	Linear elastic, slight deviation
5.2	9.0±1.5	Linear elastic, slight deviation

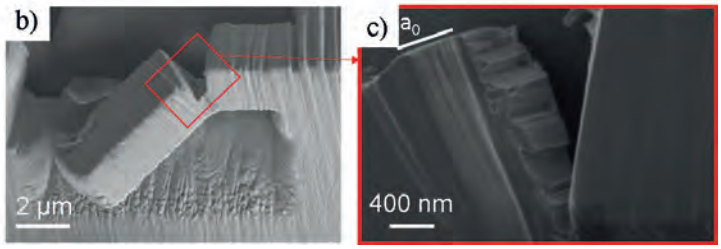

Fig. 2: *a) KIC from micro-cantilever fracture tests of cold drawn pearlitic steel wires as a function of drawing strain; b)-c) shows higher magnification images of the crack path and fracture surface.*

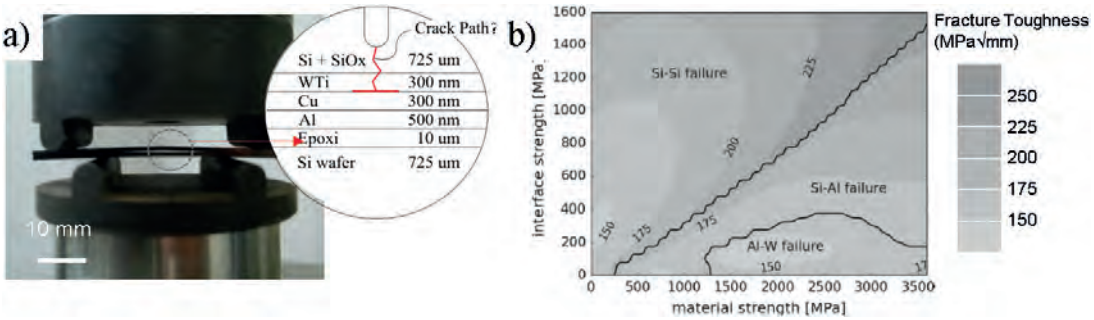

Fig. 3: *a) Four point bend fracture experiment on a MOSFET device containing multi-phase heterophase Si/SiOx/WTi/Cu/AlSiCu/Epoxy/Si interface; b) Interfacial fracture toughness map as a function of matrix and interface strengths.*

and ductile films of varying thickness (Si/SiOx/WTi/Cu/AlSiCu/Epoxy/Si) with multiple hetero-phase interfaces was examined using four point bending [5] in combination with finite element method (FEM) to evaluate the interfacial fracture energy and probability of failure (Fig 3). Results from FEM show that an optimal combination of a sufficiently weak interface architecture in a high strength matrix is beneficial for fracture toughness (Fig 3b) since it promotes crack kinking and branching and enhanced tortuosity [6]. Although common in natural materials like shell and wood, these predictions run counter-intuitive to the more common manufactured structures. FEM analysis is able to provide insights into the experimental observations in such complex scenarios, enabling lifetime predictions for multilayered systems. Currently, we are extending interface fracture experiments to a transmission electron microscope (TEM) level [7] building on our previous expertise for interface fracture testing performed at the micron-scale [8].

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Origin of Anharmonicity in fcc Materials

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The quasiharmonic approximation is nowadays the workhorse for performing thermodynamic assessments at finite temperatures using *ab initio* methods. Going beyond the harmonic picture by including the full set of relevant high temperature excitations turns out to be a daunting task. In particular, anharmonic contributions due to phonon-phonon interactions are a challenge for first principles. They cannot be considered on a daily basis due to significant computational demands: In comparison to the quasiharmonic contribution, the computational workload usually increases by more than three orders of magnitude. For this reason, studies including anharmonic contributions are rare and it is generally unknown if and to what extent they influence thermodynamic material properties. This is unfortunate, since practically relevant physical quantities as e.g., phonon life times, thermal conductivity etc. are completely controlled by anharmonicity and can only be calculated by methods which fully capture these interactions.

Until recently, only a few selected test systems were assessed by first principles methods including anharmonic atomic vibrations [1, 2]. For defects it was shown that anharmonic contributions can introduce not only qualitative but even quantitative changes to thermodynamic properties [3]. To investigate similar effects on bulk systems, we have performed a wide range study including, in particular, phonon-phonon interactions [4]. Fig. 1 compares different finite temperature contributions - such as quasi-harmonic, electronic and anharmonic - to the specific heat capacity of the investigated elements. In contrast to common belief we have found that anharmonic contributions show the same order of magnitude as the usually considered quasiharmonic contributions and that neglecting them can significantly alter the thermodynamic assessment. They can easily change phase transition temperatures by several hundred Kelvin and, as in the case of silver, significantly influence the thermodynamic stability at elevated temperatures [4].

To understand the origin of the unexpectedly large anharmonic contribution, we carefully analyzed our molecular dynamics data. Comparing the distribution of nearest neighbour vectors between two atoms for a quasiharmonic run to a fully DFT (density functional theory) based (anharmonic) molecular dynamics run we made a critical observation, which is shown in Fig. 2. While the quasiharmonic distribution (left) is seen to be fully symmetric, the DFT based run shows a distinctly non-symmetric (anharmonic) and Morse like distribution, which cannot be captured by the typically applied quasiharmonic approximation.

In a consecutive step we were able to extract the anharmonic potential from a few displacements directly at T=0K without the necessity to resort

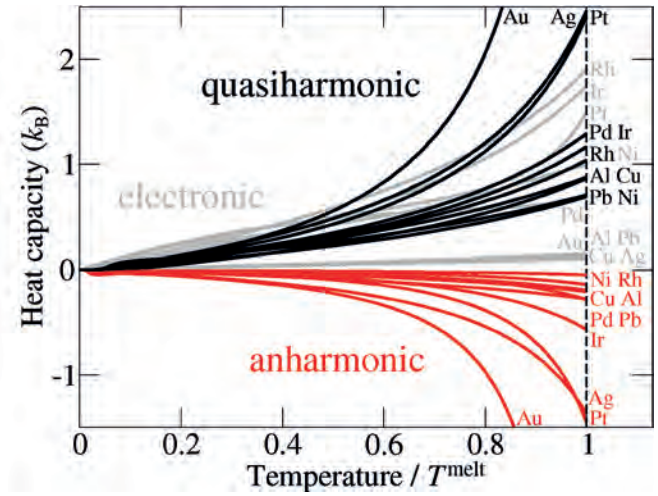

Fig. 1: *Quasiharmonic (qh), electronic (el) and anharmonic (ah) contribution to the specific heat capacity for the investigated elements as function of homologous temperature. Anharmonic contributions show the same order of magnitude as the generally considered contributions (qh and el) and their neglect can therefore significantly alter the thermodynamic assessment.*

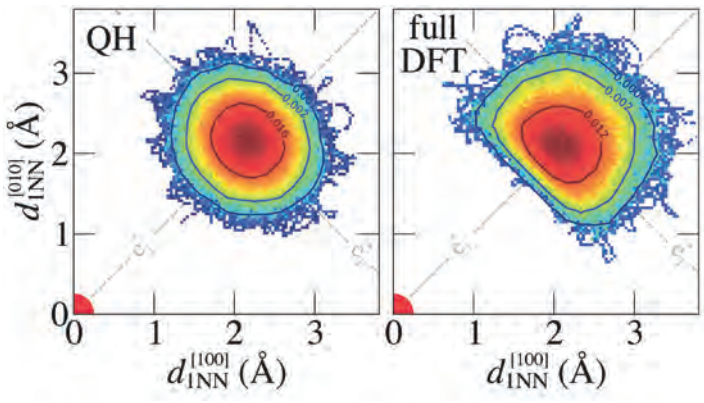

Fig. 2: *Results from a molecular dynamics (MD) run for silver at the melting temperature. For a quasiharmonic (QH, left) and a fully DFT-based potential (right), the vector between two neighbouring atoms is shown for every time step of the MD run. While the QH distribution is fully symmetric, the fully DFT based MD shows a pronounced anharmonic distribution due to Pauli repulsion. The true non-symmetric behaviour cannot be represented by a purely harmonic potential.*

to demanding molecular dynamic calculations. In particular, this was done by significantly extending the displacement range of the quasiharmonic approximation. With this we obtained a local anharmonic Hamiltonian that give rise to a new method referred to as the Local Anharmonic (LA) approximation.

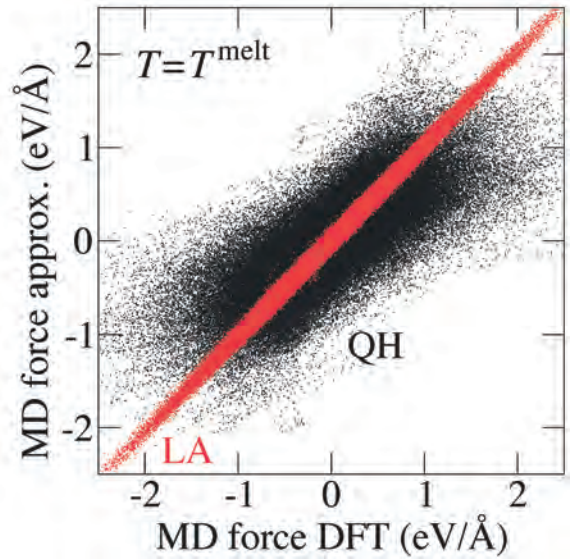

Fig. 3: *Comparison of QH (black) and LA (red) forces to fully DFT-based forces.*

Fig. 3 compares the forces of the LA (red) and the typically used QH approximation (black) to fully DFT based forces for a molecular dynamics run of Ag at the corresponding melting temperature. The LA forces are seen to significantly outperform the corresponding QH forces also for all other investigated elements (not shown). Moreover, we found that anharmonic free energies in the LA approximation deviate only by maximally 6 meV/atom at the melting point for the investigated elements in comparison to numerically exact DFT results (27 meV/atom for QH). Using the LA Hamiltonian as a reference potential for thermodynamic integration resulted in a typical speed up of two orders of magnitude in comparison to the QH reference. This opens the path towards routine, numerically exact *ab initio* free energies. First assessments of phonon line widths using the LA approach seem very promising and are currently investigated in detail.

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Grain Boundary Embrittlement in Fe-Mn Alloys

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Medium manganese steels are binary base model alloys for a third generation of high strength steels [1]. Excellent mechanical properties are mostly related to the TRIP effect, which arises due to the presence of reverted austenite in the microstructure. Unfortunately, these alloys are brittle in the compositional range of interest between 5 to 12 at% Mn [2 - 4]. This embrittlement becomes particularly pronounced in the impact toughness test even at room temperature. Fig. 1 shows that even a tempering treatment as short as 10 s is sufficient to embrittle prior austenite grain boundaries (PAGBs).

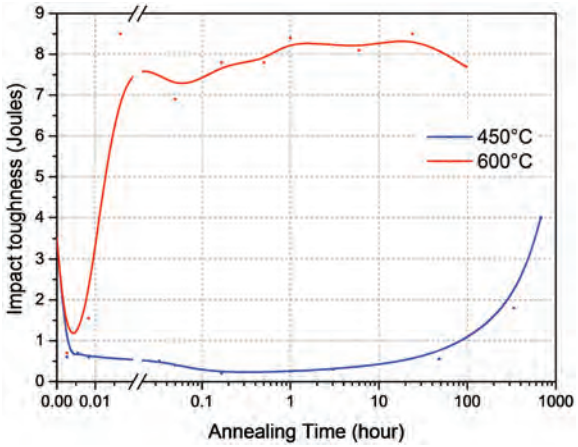

Fig. 1: *Fe-9wt%Mn, Impact toughness at room temperature after tempering at 450 °C and 600 °C and subsequent quenching.*

Segregation induced grain boundary (GB) embrittlement is a common reason for a decrease of grain boundary cohesion. To analyse the segregation on an atomic level atom probe tomography (APT) was applied on site specifically FIB (Focused Ion Beam) prepared PAGBs after different heat treatments. Atom distribution maps and corresponding concentration profile is plotted in Fig. 2 for an embrittled case after a short tempering at 450 °C. The increase of Mn concentration without a significant change in concentration of other elements indicates that Mn segregation can be associated with the temper embrittlement.

In order to get an unambiguous proof for the Mn effect on GB embrittlement, further APT measurements of GB chemistry in de-embrittled state after long tempering times were performed. For an evaluation of PAGB concentrations GB excess values were extracted and plotted in Fig. 3. A rapid increase in Mn excess value after tempering at 450 °C is followed by a decrease after prolonged tempering time. The Mn excess value curve has an excellent correlation to the impact toughness values: thus a GB embrittlement is caused by an increase of a Mn excess value and a further improvement of impact toughness corresponds with a decrease of the Mn excess values. This decrease of Mn excess value is attributed to a formation of Mn-rich austenite phase on GBs and consumption of Mn from the GBs, hence cleaning them from Mn segregation.

In order to understand the underlying mechanisms for Mn induced GB embrittlement, *ab initio*

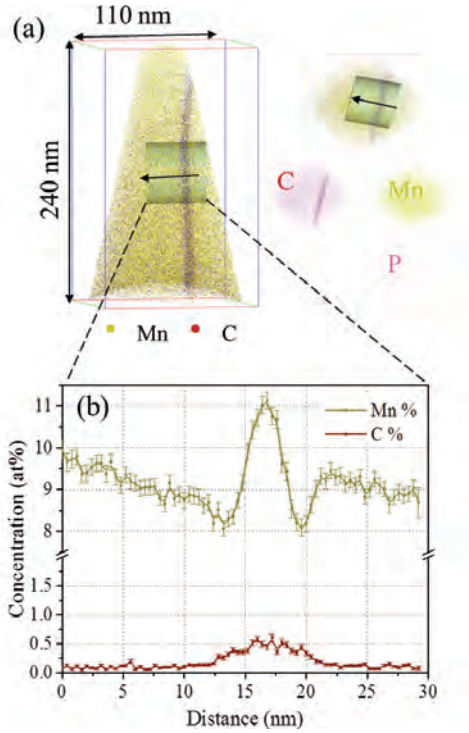

Fig. 2: *(a) APT results obtained on Fe-9wt% Mn tempered at 450 °C for 1 min. 3D side view and top view of the dataset of the same region, with the corresponding element distribution maps revealing the accumulation of C, Mn on the PAGB and a homogeneous distribution of P; a corresponding 1D concentration profile (b) shows enrichment of C and Mn atoms.*

calculations based on density functional theory as implemented in the Vienna *ab initio* simulation package (VASP) have been performed. In a two-step approach, we first analyzed the behaviour of Mn in bcc Fe, considering supercells of 54 atoms. To model in a second step the Mn segregation at grain boundaries, the ∑5(013) GB has been simulated in a 120 atoms supercell. This is a tilt GB constructed

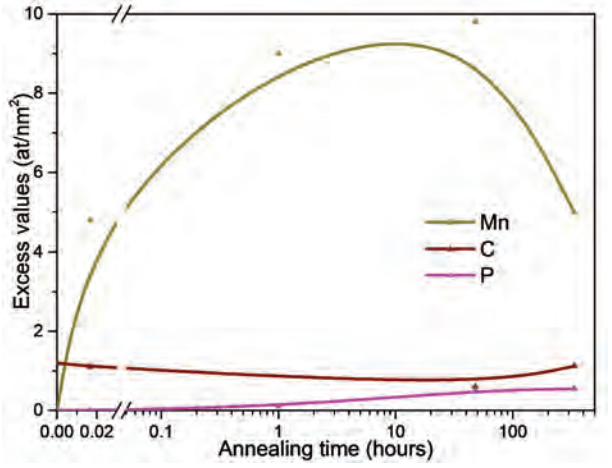

Fig. 3: *An evolution of manganese, carbon and phosphorous grain boundary excess values after tempering at 450 °C.*

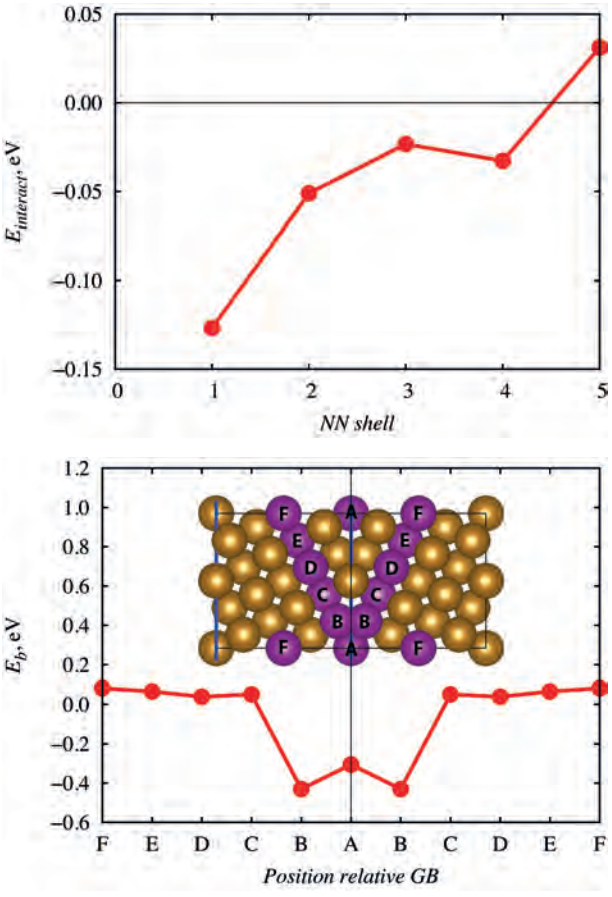

Fig. 4: *(a) Effective interaction energy between two Mn interstitials in bcc Fe as a function of their separation and (b) Segregation energy of Mn interstitial as a function of distance from the boundary plane (the insert shows the structure of the symmetrical ∑5(013) grain boundary).*

using the coincidence site lattice (CSL) approach by rotating two bcc lattices by 36.9° around the [100] direction, see Fig. 4.

The calculations with one Mn solute atom in bulk ferromagnetic (FM) bcc Fe revealed the preference for Mn to have a local magnetic moment antiparallel to those of the surrounding Fe atoms. A clustering of Mn atoms could therefore be stabilized by a change of the magnetic ordering to an antiferromagnetic (AFM) configuration. An effective interaction energy depending on the distance d between two Mn atoms, $E_{interact}(d) = (E_{Mn+Mn}(d) + E_{bcc}) - (E_{Mn} + E_{Mn})$, characterizes the solute-solute interaction in a bcc supercell. Here, the total energy of the cell containing two substitutional Mn atoms (E_{Mn+Mn}) is compared to those of supercells without Mn (E_{bcc}) and with one Mn atom (E_{Mn}). From Fig. 4a one can see that Mn has local clustering tendency in bcc Fe ($E_{interact} < 0$) at 0K (compare [5]).

The tendency for the individual Mn atoms to segregate at a grain boundary is described by the binding energy: $E_b = (E_{Mn+GB} + E_{bcc}) - (E_{GB} + E_{Mn})$, where E_{Mn+GB} and E_{GB} are the total energies of the supercells containing grain boundaries with and without a Mn atom, respectively. A negative value of E_b indicates an attraction of the solute atom to the GB. From Fig. 4b one can see that Mn atoms prefer position B (see insert in Fig. 4b) - not exactly at the GB but the atomic sites nearest to the boundary plane.

Thus, the observations obtained so far by our zero K calculations indicate that the following mechanisms could support the grain boundary embrittlement: Firstly, Mn has a tendency to segregate near the GB. Secondly, the attractive interaction between Mn atoms in bcc Fe supports the clustering of Mn atoms in this region. Thirdly, the antiferromagnetic interaction of the Mn atom will yield a change of the magnetic ordering where Mn clustering occurs. It is known also that AFM lattice constant differs from that of FM state. Therefore, Mn segregations on grain boundaries may serve as strain concentrators in medium-Mn steels.

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Impact of Anharmonicity and Nonlocal Many-Body Effects on the Thermodynamics of Au

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Theoretical efforts at the MPIE over the past years have provided various techniques for computing thermodynamic properties from *ab initio*, thereby greatly contributing to our understanding of finite temperature materials properties. Mostly, these developments were based on standard approximations to the exchange-correlation functional within density-functional-theory (DFT). For a wide range of materials these approximations provide an excellent description of finite temperature properties up to the melting point as the CM has shown previously (see p. 46). However, standard functionals are known to have intrinsic deficiencies, e.g. for elements with nearly full electron shells such as Au. In fact, the heat capacity of Au computed within the generalized gradient approximation (GGA) shows even a diverging behaviour, well below the experimental melting temperature regardless of whether anharmonicity is included or not (orange solid and dashed grey line in Fig. 1).

In collaboration with Dr. Stefan Wippermann (GO), we have recently extended our previous thermodynamic approaches allowing now to compute finite temperature properties, in particular anharmonicity, at a level beyond the standard approximations [1]. For that purpose, we have coupled the upsampled thermodynamic integration using Langevin dynamics (UP-TILD) method [2] with the random phase approximation (RPA) employing the adiabatic-connection-fluctuation-dissipation theorem [3]. This new RPA UP-TILD technique allows to investigate the impact of nonlocal many-body effects on thermodynamic properties, and for Au we could show that the severe discrepancies introduced by the standard functionals disappear (green line in Fig. 1) and that an excellent agreement with experiment is obtained (black dots).

The crucial challenge in developing the RPA UP-TILD method was to overcome the prohibitive computational workload which would arise if the RPA technique was coupled directly to state-of-the-art molecular dynamics simulations. To this end, we followed a perturbative strategy as in the original UP-TILD method. In particular, within RPA UP-TILD, we utilize a molecular dynamics simulation performed within standard DFT, e.g. using GGA, to obtain a phase-space sampling at the desired volume and temperature. We then extract a few uncorrelated snapshots and calculate the RPA UP-TILD energy as

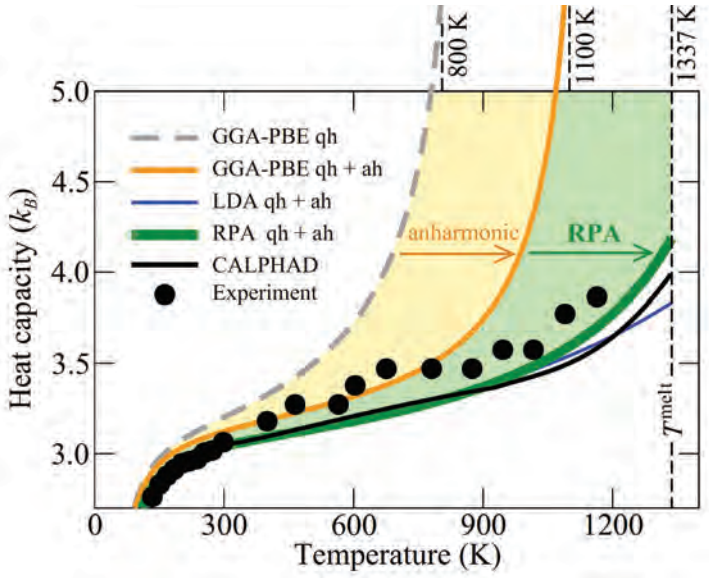

Fig. 1: *Application of the new RPA UP-TILD method to Au. Using the generalized-gradient-approximation (GGA) a diverging heat capacity is obtained, regardless of whether the standard quasiharmonic (qh) approach is used (grey dashed line) or the state-of-the-art extension to anharmonic (ah) contributions (orange solid line). It is only upon application of the newly developed RPA UP-TILD method (green solid line) that a good agreement with experiment (filled circles, Ref. [4]) is obtained. Figure adapted from Ref. [1].*

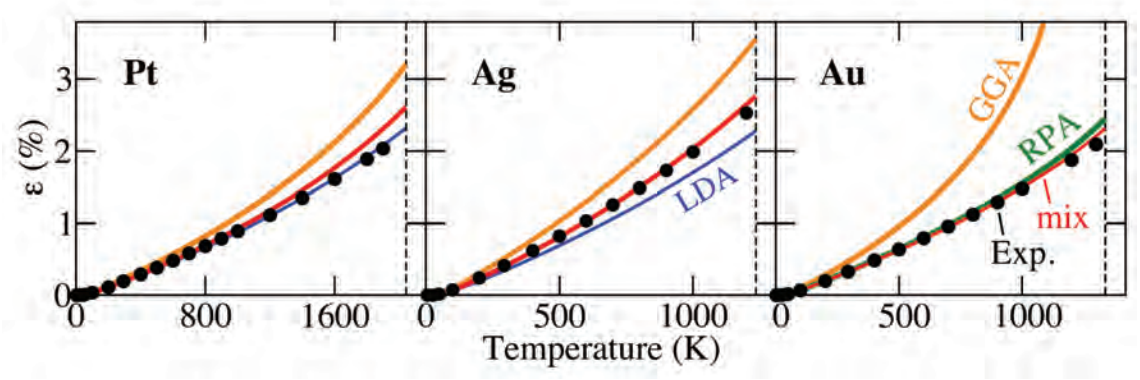

Fig. 2: *Linear thermal expansion calculated within GGA (orange lines; including anharmonicity), fully within RPA obtained with the here introduced RPA UP-TILD method (green line; Au only), and using a mixed approach (red lines) employing the T = 0 K RPA curve in conjunction with GGA-PBE finite temperature excitations. Experimental values (solid circles) are from Ref. [8].*

a difference between the GGA and RPA energies of the corresponding supercell. Adding this difference to the T=0 K RPA energy and to the GGA vibrational free energy, we obtain the total free energy with an accuracy of the RPA method.

A strength of the developed RPA UP-TILD methodology is that the different contributions can be investigated separately. Our analysis has shown that the strong impact of RPA (green shaded region in Fig. 1) originates mainly from differences in the T = 0 K energy-volume curves and corresponding values for the equilibrium lattice constant and bulk modulus. The GGA values (4.15 Angstrom and 140 GPa) are substantially modified by the RPA (4.10 Angstrom and 175 GPa) giving rise to a considerably stiffer bulk. This stiffness is the factor responsible for shifting the divergence in the thermodynamic quantities beyond the experimental melting point.

Utilizing this insight, we have proposed an efficient approach to compute accurate finite temperature properties beyond standard DFT. The approach combines T = 0 K RPA energies with entropic contributions from standard exchange-correlation functionals such as GGA. Applying this approach, we obtained, with little computational effort, RPA finite temperature results for Ag and Pt, the elements showing the largest discrepancies within GGA except for Au [5]. As shown by the red lines in Fig. 2, the mixed approach provides excellent agreement with experiment for all studied elements and with full RPA for Au. This indicates that nonlocal many-body effects as captured by RPA affect predominantly the absolute binding energies at T = 0 K, while thermal vibrations are unaffected to a good approximation.

The insensitivity of high-temperature vibrations to nonlocal many-body effects is remarkable since recent studies [6] showed that close to melting the displacement of atoms from their equilibrium positions is significant and that the first-neighbour distance distribution is strongly affected by anharmonicity. Knowing that the GGA deficiency is not related to thermal vibrations but rather to the T = 0 K energy surface indicates a possible route for the development of accurate *ab initio* databases. T = 0 K computations are generally efficient since small supercells for single (or at most a few) atomic configurations are sufficient. It becomes therefore possible to employ computationally elaborate alternatives, such as the RPA technique employed here, to supplement the databases.

The introduced technique is not restricted to a combination of standard DFT with RPA. Any other higher level approach (e.g., quantum Monte Carlo [7]) can be coupled to standard DFT and used to obtain the accurate energies for the UP-TILD instead of the RPA.

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Magnon-Phonon Coupling at Arbitrary Finite Temperatures

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An understanding of the mutual interaction between different temperature-induced excitations in solids is a pivotal challenge for the simulation of thermodynamic properties of many materials [1-3]. A particularly important interaction is the interplay between magnetic and atomic degrees of freedom, building the basis for many methodological applications [1]. For Fe-based materials, it is well known that magneto-elastic effects are of tremendous importance for the interpretation of various phenomena such as the Invar effect, diffusion processes, dislocation dynamics, and phase stabilities [1-3].

Density functional theory in principle provides access to interatomic forces, spin-polarized energetics, and their interactions. Force-constant calculations and spin simulations have been performed for decades. However, most studies have been restricted to separate investigations of the two effects, whereas their mutual coupling could only be addressed in recent years [1-4]. The T=0 K limit of a ferromagnetic system like Fe is the most straightforward case since calculating force constants for a single magnetic configuration with all spins pointing in the same direction is sufficient ("FM limit" in Fig.1). The infinite-temperature limit of a paramagnetic system with fully disordered spins ("PM limit") is significantly more challenging due to the large magnetic phase space that needs to be sampled for an accurate prediction of the coupling. Significant progress has been made only very recently with techniques based on, e.g., the disordered local moment molecular dynamics (DLM-MD) or the spin-space averaging procedure (SSA) [3,4].

At high temperatures, the DLM-MD and the SSA have both been equally successfully applied to describe phase stabilities in complex alloys such as recently shown for instance on the industrially important CrN system [3,4]. However, given the complexity of the problem, current methods are accurate only at very low temperatures, where significant long-range order is present, and at very high temperatures, where the system has lost all order in the spin arrangement. Intermediate temperatures are not directly accessible by explicit DFT calculations as prohibitively many large supercells would be needed to properly capture the partially destroyed long-range order and the inhomogeneously scattered regions with short-range order.

We therefore developed and applied a method that employs a set of DFT calculations carried out for only the FM and PM limits in conjunction with quantum Monte Carlo sampling (see e.g. [1]) to obtain properties at intermediate temperatures. The method is capable of describing magnon-phonon coupling at arbitrary finite temperatures, closing the previous simulation gap between the T=0 K and high-temperature limits. The performance of the method is demonstrated in Fig. 2, wherethe calculated temperature dependence of the phonon frequencies in bcc Fe is compared with experimental measurements (filled black squares in Fig. 2). The approach has been further validated by a new set of phonon frequencies measured at 38 temperatures (open circles in Fig. 2) by our experimental collaborators at the Advanced Phonon Source in Argonne [5]. The excellent agreement

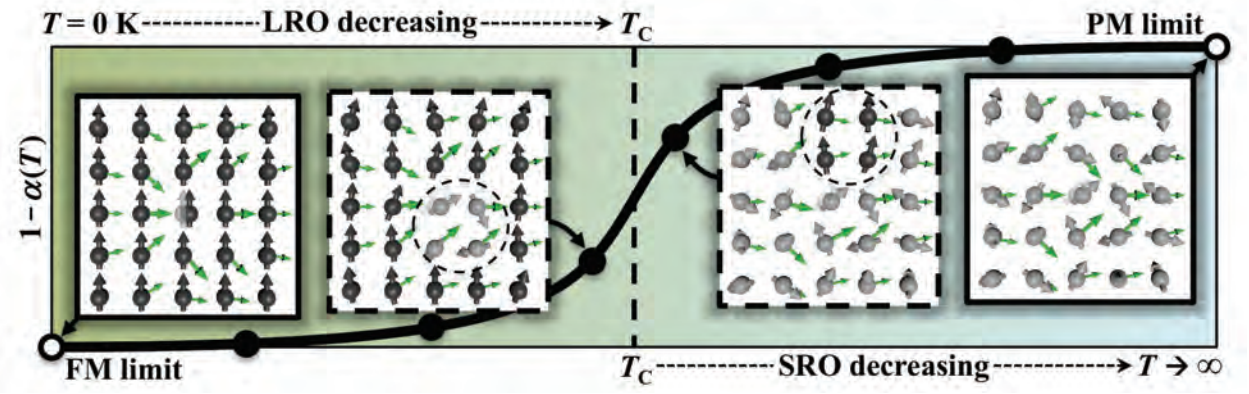

Fig. 1: *Sketch of the developed method coupling the energetics of the magnetic system with explicit DFT force constant calculations (displaced spin in the middle of each sketch). The gray and green arrows indicate the local magnetic spins for each atom and the interatomic forces (restoring forces when 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.*

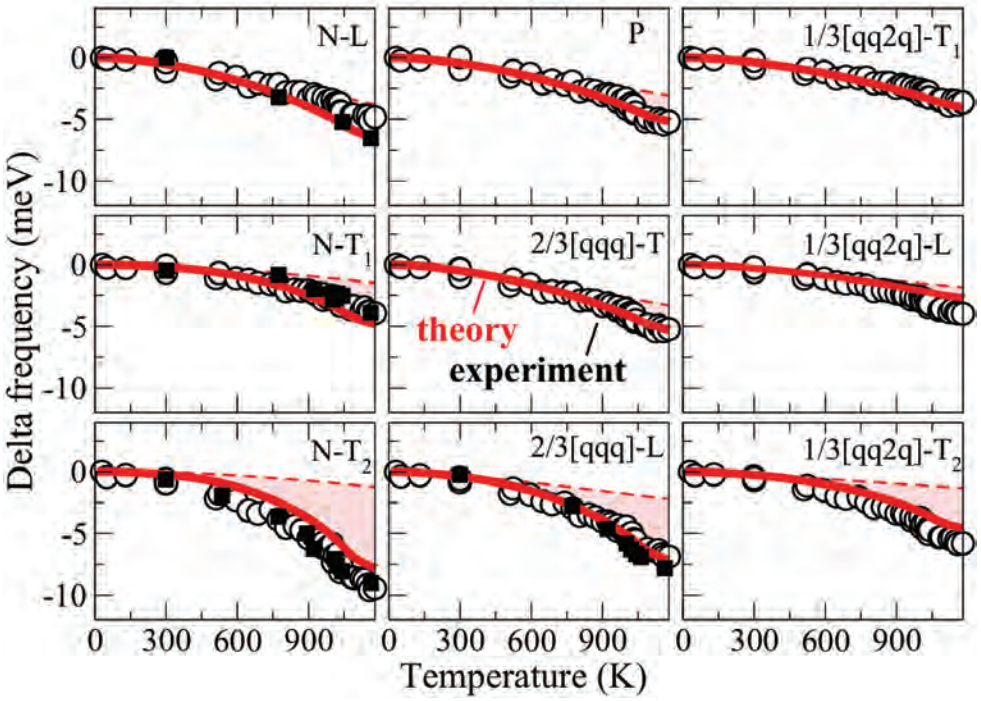

Fig. 2: *Temperature dependence of phonon frequencies for different modes comparing theoretical (solid red lines) with experimentally deduced frequencies (open circles). Dashed red lines show the ferromagnetic quasiharmonic results (no phonon-magnon coupling). Where available, previous neutron scattering data are included (filled black squares).*

between theory and experiments provided new insights into the role of magnon-phonon contributions for the thermodynamic stability of iron.

Going from elemental iron towards more complex Fe-based alloys, coupled chemical and magnetic order-disorder transitions need to be simultaneously taken into account. For this reason we have recently extended the SSA method by constructing chemical and magnetic random supercells, and performing complementary magnetic Quantum Monte Carlo simulations. The application to Fe-based Invar alloys shows indeed a similar agreement for temperature-dependent atomic excitations with experimental data as obtained for pure iron [6].

A present challenge for the DLM-MD and SSA techniques is still the inclusion of the so-called longitudinal magnetic degree of freedom (i.e. the variation of the magnitude of local magnetic moments) and particular its coupling to the atomic motion. On the one hand, for magnetic systems such as iron, which show rather "robust" local magnetic moments, atomic vibrations still impact the longitudinal spin degree of freedom by distorting local atomic geometries at high temperature. One effect is the induction of a spatial variation of local moments and a temperature dependence of their mean value. This is currently being investigated by employing the DLM-MD for paramagnetic gamma and delta iron [7]. On the other hand, for magnetic systems known for strong local moment fluctuations such as, e.g., Nickel, we have further extended the SSA by combining it with constrained spin DFT [8].

The complementary developed techniques allow us thus to investigate phonon-magnon contributions for a large class of magnetic systems, ranging from weak to strong ferromagnets as well as from elemental magnets to complex magnetic alloys. We anticipate that their future unification will allow quantitative modeling of the stability and properties of magnetic materials for temperatures ranging from 0 K up to the melting point.

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Tribology across the Length-Scales

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Tribology occurs in almost all applications of metals when two surfaces get into contact. Friction and wear occur on multiple hierarchical length-scales, on each of which different mechanisms interact. On the macroscopic length-scale, the dynamics of elasticity and friction are investigated. We study plasticity, crack formation and surface roughness evolution on the micrometer length-scale. Friction and irreversible atomistic processes are researched on the nanometer scale.

On the atomistic length-scale at the surface, tribological processes in aqueous and corrosive environments are studied. The central crosslinking aim of this work is to understand the multiscale nature of wear and friction by upscaling from the nanometer to the micrometer length-scale. Therefore, friction experiments are performed with both atom force microscopy (AFM) and surface force apparatus (SFA) at the nanoscale. During single-stroke scratching in the nano-Newton regime, no irreversibility is visible at the given scale, as shown in Fig. 1.

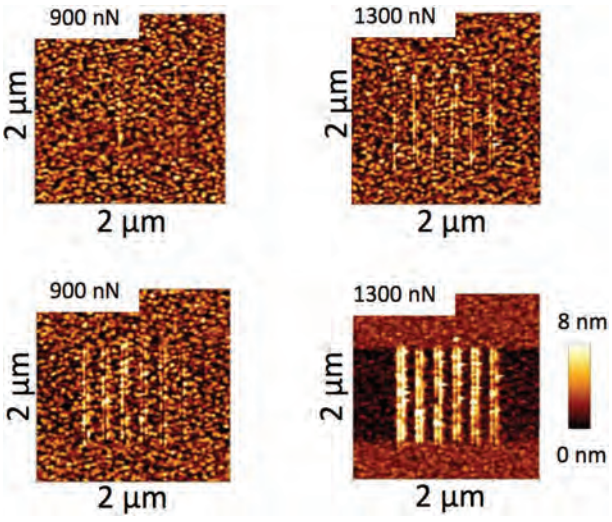

Fig. 1: *Top row: nanoscopic single stroke scratch tests with an atomic force microscope (AFM) at 900 nN and 1300 nN applied normal force. Bottom row: 10 stroke scratch tests reveal critical damage onset on the nanoscale. The vertical scale is identical in all images.*

However, when repeating the strokes, damage and the scratch tracks become visible. These dry friction and wear measurements are combined with studying the molecular structuring of lubricants in both aqueous and non-aqueous lubricants. In particular, on the material surface interfacial structuring of lubricant molecules (electric double layers, layering of lubricants are measured at the atomistic scale in order to correlate lubricant structuring and material properties with friction and wear performance. Combining these efforts with the complementary set of experiments in the other departments will pave the road for understanding friction and, in particular, wear and damage over all length scales.

Even polished surfaces have a microstructural roughness that leads to the microasperity contact when engineering surfaces get into contact. In the experiments, the nanoindenter with lateral force measurement is used to mimic friction and wear of a single microasperity. To this end, a hard spherical tip is scratched through the bulk metal and the plasticity on the track sides and in front of the scratch is investigated. The crystal orientation plays the dominant role in determining the slip pattern around the scratch track and the development of surface roughness. Grain boundaries act as partial obstacles to the transfer of plasticity: a subset of the plasticity causing dislocations is blocked at the grain boundary while the other dislocations penetrate the grain boundary. The massive dislocation plasticity at the surface ahead of the microasperity results in the formation of subsequent surface roughness and finally crack formation in the scratch track. The stress state in the scratch track is three-dimensional and results in mixed mode crack growth.

On the micrometer length-scale, crystal plasticity simulations with the DAMASK toolkit are used to further the understanding of plasticity around microasperities. The three dimensional stress state around the dynamic asperity is influenced by the crystal orientation and anisotropy of the material. Moreover, the proximity of grain boundaries restricts the plasticity. Hence, Finite Element Simulations of the crystal plasticity are warranted that take into account the contact of asperity and surface and evolve the contact as the asperity moves along the surface. To this end, the indentation and then horizontal movement of an infinitely hard sphere through an austenite counter material is simulated and the height-profile around the asperity is plotted. The severe plastic deformation around the asperity shows distinct differences when scratching in grains of different orientation and these slip surface patterns are similar to the experimental results: severe plasticity occurs around scratches in [111] oriented grains, as shown in Figs. 2 and 3.

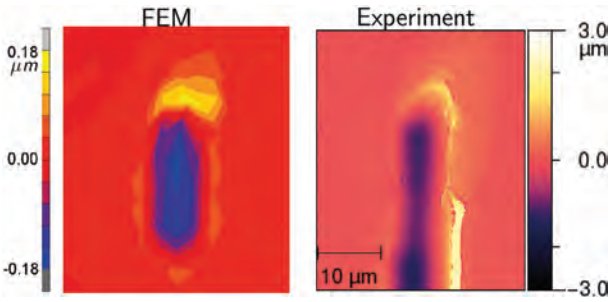

Fig. 2: *Qualitative comparison of crystal plasticity finite element (FEM) simulations and experiments on the microscale. The pile-ups ahead of the scratch are tilted slightly to the right-hand side. The height profile is shown in both images for an austenite grain with a surface normal close to the [111] orientation. Because of differences in length-scale, differences in the height occur.*

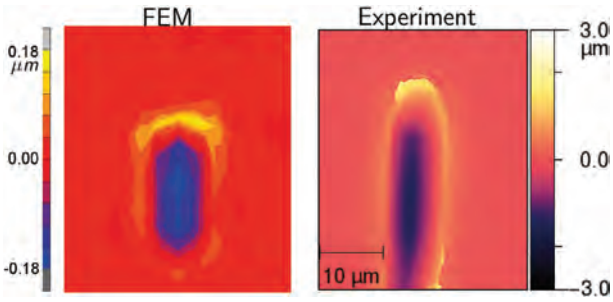

Fig. 3: *Qualitative comparison of FEM simulations and confocal measurements of a scratch in an austenite grain close to the [101] normal orientation. The pile-ups ahead of the scratch are almost straight and have a short extension. Differences in the height occur because of differences in length-scale and differences in scratch depth.*

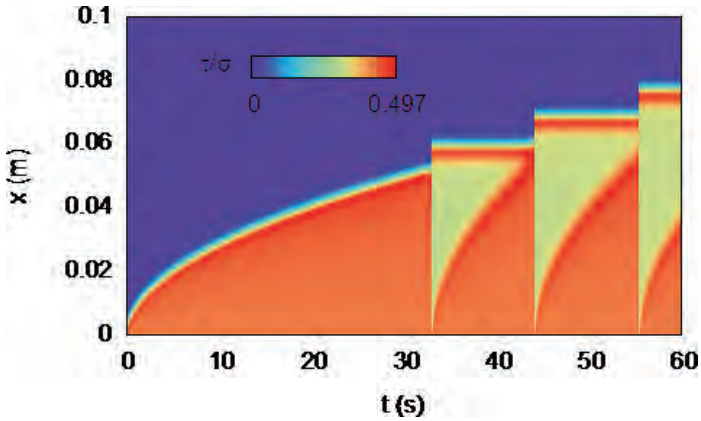

Fig. 4: *Space-time plot of the frictional stress at the contact surface between a rigid substrate and a slider. The red parabolic region corresponds to the slow propagation of a creep patch, which then repeatedly triggers "fast" events. The inset shows the slow-motion view with a detachment front velocity of only 3.3 m/s, which is much lower than the shear wave speed.*

Irreversible effects on the microcontact level during dry surface sliding contribute to the microasperity ageing. This aging microcontacts lead to velocity weakening of the macroscopic dynamic friction coefficient as function of sliding velocity. Rheological and chemical effects, in turn, favor the opposite effect of velocity strengthening [1]. The combination of velocity weakening and strengthening lead to minima of the frictional force as function of velocity, as we have shown recently in an extended survey of experimental data [2]. Near this minimum "stick-slip" pulses can propagate with velocities orders of magnitude lower than the speed of sound [3], which is a potential explanation for laboratory and geological observations of "slow earthquakes", as shown in Fig. 4. These slow propagation waves are emitted from creep patches, which are localized weakening precursors at the interface under shear, which become unstable after a certain propagation distance and trigger detachment front propagation [4].

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Linear and Planar Complexions: Confined Chemical and Structural States in Steels

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Medium manganese steels are of high scientific and commercial interest as they combine high strength and ductility with low material costs [1]. The mechanical properties are mostly related to the TRIP (Transformation Induced Plasticity) effect, which arises due to a presence of reverted austenite in the microstructure. Improving material properties requires a deep understanding of the underlying phase transformation and deformation mechanisms. In a binary martensitic Fe-9wt%Mn alloy with very low carbon content (75 wt. ppm) we observe a serrated appearance of the stress-strain curve at 450°C as well as a discontinuous yielding after tempering at 450 °C for 6 hours. These phenomena have so far mainly been observed in the Fe-C system, where they are referred to as dynamic and static strain ageing, respectively.

Here we investigate this effect using tensile tests, coupled to correlative transmission electron microscopy (TEM) and atom probe tomography (APT) characterization [2–4], performed exactly at the same location to gather direct evidence for the interaction of solute atoms with dislocations.

Fig. 1 depicts such a correlative TEM/APT analysis performed on the material that had been 50% cold-rolled and tempered at 450 °C for 6 hours. Two grain boundaries and a single dislocation line, highlighted by blue arrows, are visible in the TEM image through Bragg contrast and in the 3D atom map in the form of Mn-enriched regions. Not all dislocations visible in the STEM micrograph cause segregation that is sufficiently high to be detectable by APT (red arrow 1) and vice versa (red arrow 2). Calculation of the interaction energy between a Mn atom and both, an edge dislocation and a screw dislocation reveal that Mn has a strong tendency to segregate to edge dislocations. Atom probe crystallography methods confirmed that all the observed dislocation lines have edge character [5].

Strong segregation in conjunction with pronounced local elastic distortions may promote phase transformation [6]. The level of segregation on some dislocations in the tempered Fe-9wt%Mn alloy reaches 25 at% Mn, which is the equilibrium concentration of Mn in austenite at this tempering temperature [7]. TEM analysis, performed on a thin foil, provides direct evidence for the presence of a new structural state localized at an edge dislocation in a dark field view in Fig. 2.

If a new structural state with a 1-2 nm diameter is formed, its growth would be expected during longer tempering times. However, when the sample was tempered for 336 hours at 450°C and analysed, neither growth of the segregation zone nor changes in concentration were observed. This result indicates that in this special case of heterogeneous nucleation at dislocations the critical radius for a viable austenite nucleus is not yet reached.

The observed formation and confinement of austenite is determined by the dislocation stress field. Without dislocations, small size austenite nuclei are thermodynamically unfavourable due to the endothermic interface energy between austenite and the surrounding martensite. However, in the vicinity of the dislocation core, the volume change that is associated with the transformation of martensite into austenite partly compensates the strain energy induced by the dislocation and renders the transformation energetically more favourable. This effect is stronger

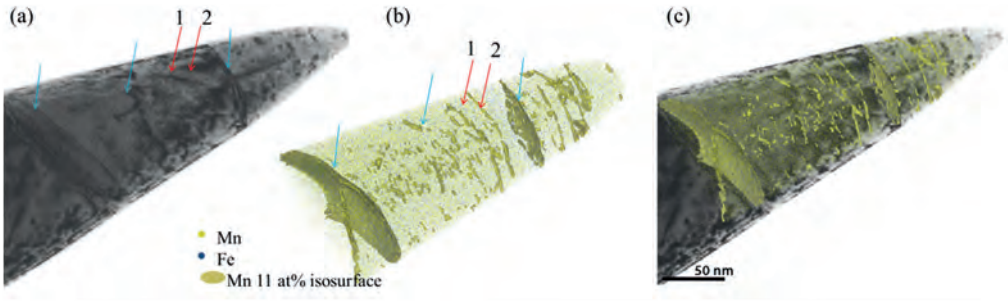

Fig. 1: *Fe-9wt%Mn, 50% cold-rolled and tempered at 450 °C for 6 hours to promote Mn segregation; (a) TEM image; (b) Atom probe tomography results; (c) Overlay of both, TEM and APT; Iso-concentration surfaces indicate areas with Mn concentrations above 11 at%. The blue arrows mark grain boundaries and dislocation lines that are visible in both, the TEM micrograph and the atom probe tomography map.*

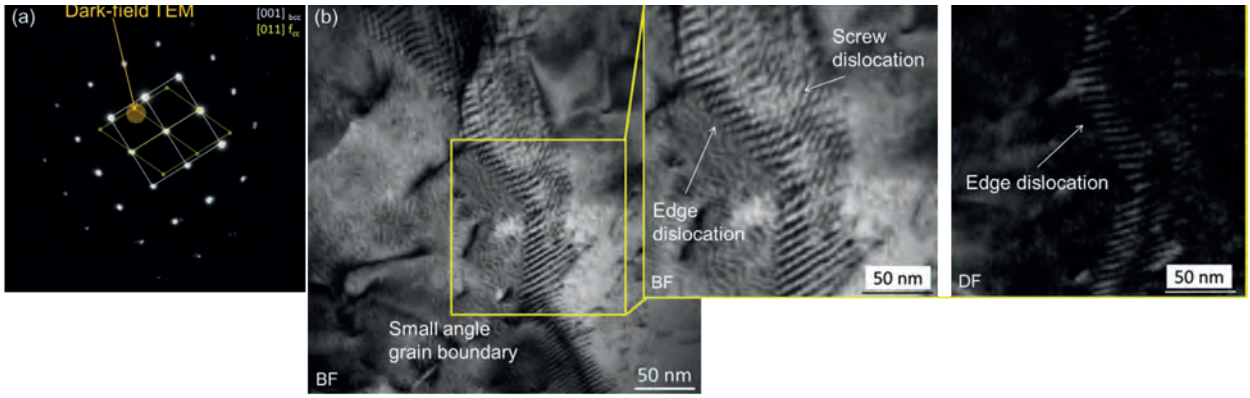

Fig. 2: *(a) Selected area diffraction pattern (SADP) from the enlarged region shown in Fig. 2(b), the diffraction pattern is indexed as $[001]_{bcc}$, the positions of the fcc diffraction spots for a N-W orientation relationship are drawn into the image. (b) Bright-field and dark-field TEM micrographs of a small angle grain boundary, the dark-field micrograph was taken from the region marked by the dark-yellow circle in Fig. 2(a).*

at small diameters and gradually decreases as the diameter increases. As a result, the local transformation is favourable at small diameters but its growth is arrested at some equilibrium diameter (Fig. 3).

A direct simulation of this phenomenon is computationally difficult due to the wide range of the length-scales (long-range dislocation stress field, short range solute-solute interaction) and time-scales

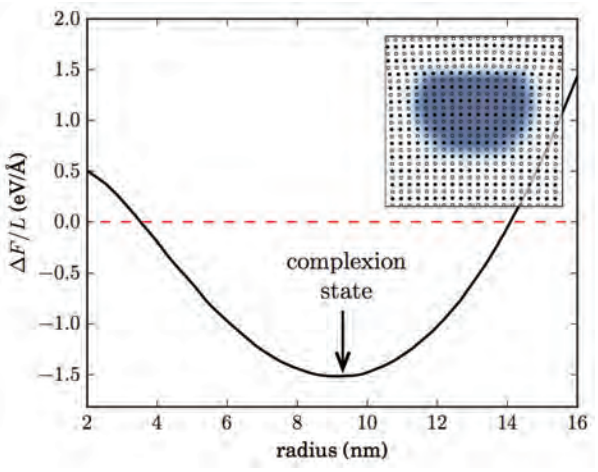

Fig. 3: *The Free energy change per unit ΔF/L of a cylindrical complexion with radius r around an edge dislocation. The examples shown here are for a NiH system at 300K and a bulk hydrogen concentration of 60ppm.*

(diffusion) involved. To address this, we have developed a multiscale modelling approach that couples an analytic model with atomistic calculations to eliminate arbitrary fitting parameters [8]. This approach has been successfully applied to predict and quantify the phase space where dislocation stabilized hydride complexions formed in the Ni-H system (e.g. Fig. 3). The formalism will be extended in a next step to the Fe-Mn system discussed here.

Such a confined structural and chemical state is phenomenologically similar to the term complexion used in the literature [9–11]. Up to now the term complexion has been used only for planar defects such as grain boundaries, where the driving force for complexion formation lies in the reduction of the interface energy. Using *ab initio* simulations, we have shown that these phenomena are also present at dislocation cores surrounded by a ferrite-austenite interface in Fe-based materials [12]. We thus extend this term to the linear case, which is driven by the high dislocation line energy reduction associated with the segregation and a subsequent formation of distinct confined structural states [13].

We have demonstrated for the first time the formation of linear complexions along dislocation lines in a model Fe-9wt% Mn steel. These observations extend the method of segregation engineering via complexions to the linear case, opening up new opportunities to control the microstructure on a nanoscale level.

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Deformation-Induced Martensite in Severely Cold-Drawn Pearlitic Steel: A New Mechanism at Play

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Cold-drawn pearlitic steel wires exhibit ultra-high tensile strengths of up to 7 GPa [1] being thereby the world's strongest bulk materials, used for a wide range of applications such as suspension bridge cables, springs and tire cords. The high strength of cold-drawn pearlitic steel wires has been associated with the refinement of the originally lamellar eutectoid iron-cementite structure of the pearlite during the wire drawing process, but also with other relevant mechanisms including cementite dissolution and the formation of nanoscale dislocation substructures [2-4]. Upon heavy cold drawing the carbon atoms are released from the dissolving cementite [1,2] and are mechanically alloyed into ferrite. The carbon concentration in the ferrite phase dramatically exceeds the equilibrium solubility limit. In this work, we show that carbon inside the ferrite grain interiors causes a lattice distortion indicating a deformation-driven phase transformation from BCC ferrite to BCT martensite. A new theory based on *ab initio* calculations confirms that such a structural transition takes place by Zener ordering.

Using atom probe tomography (APT) the accurate quantitative carbon concentration in solid solution was analysed at various drawing strains ε. Synchrotron X-ray diffraction was applied to characterize the evolution of lattice parameters, texture and strain in the ferrite phase with respect to the evolution of the carbon concentration. In parallel, we conducted density functional theory (DFT) calculations to elucidate the physical origin of the drawing strain effect on the structural transition of the ferrite phase.

Fig. 1a shows the measured carbon concentration versus the drawing strain for both nominal compositions studied. We find out that the drawing process induced a significant increase in the carbon content inside the originally near-carbon-free ferritic lattice until a steady state is reached at ε ≥ 4. The corresponding evolution of the lattice parameters of the initial ferrite phase with increasing drawing strain is shown in Fig. 1b.

Clearly, the initial bcc lattice of the ferrite unit cell becomes tetragonal distorted with increasing drawing strain (ε ≥ 2). The distortion increases with increasing drawing strain as shown in Fig. 1b. This observation holds true for both, initially eutectoid and hypereutectoid compositions. Fig. 1b reveals three

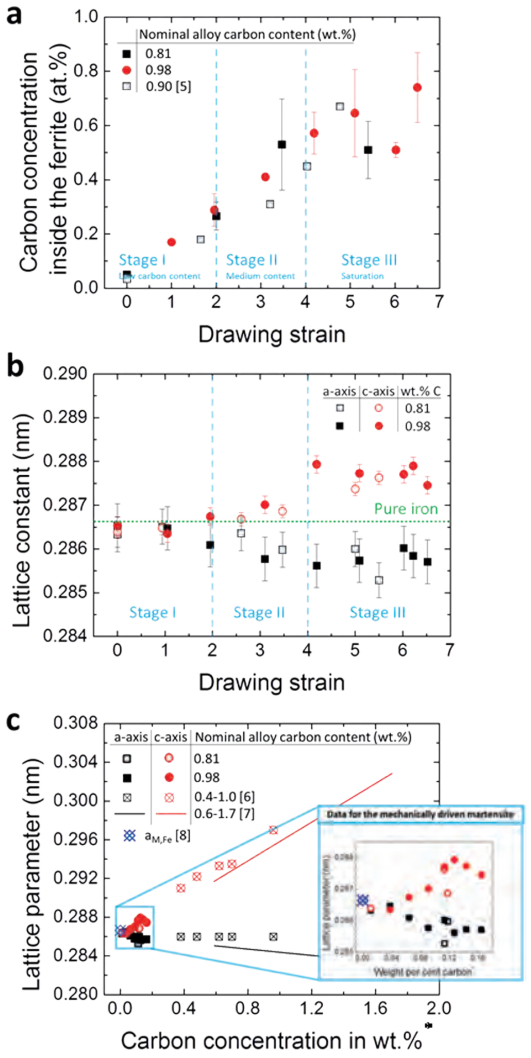

Fig. 1: *(a) Carbon concentration inside the ferrite grain interiors for pearlite wires with different nominal alloy carbon concentration. Literature data [5] for hypereutectoid (0.90 wt.% C) pearlitic steel are used for comparison. (b) Lattice parameters along a-axis and c-axis of α-ferrite lattice during the drawing process. The green line corresponds to pure iron. Blue lines highlight the different stages of structure evolution. (c) Lattice parameters a and c of conventional as-quenched martensite with different nominal (i.e. global) alloy carbon content (cross symbols and solid lines) taken from the literature [6] and [7], plotted together with our data (open and filled symbols, a zoom of them is shown in the inset). aM,Fe refers to the lattice parameter of martensite in carbon-free iron [8]. The asterisk * in the abscissa axis is added to underline the difference between the carbon content of the present study measured by APT in the ferrite grain interiors and those taken from literature referring to the nominal carbon content.*

stages in the evolution of the lattice parameter with drawing strain. In stage I ($\varepsilon < 2$), the ferrite unit cell has a bcc crystal structure where the lattice parameter remains unchanged and is equal to that of pure iron. In stage II ($2 \leq \varepsilon \leq 4$), the lattice parameter splits into two values corresponding to a tetragonal structure with two different axes a and c. Up to $\varepsilon = 4$, the a-axis shrinks by ~ 0.36% while the c-axis is expanding by ~ 0.45%. In stage III ($\varepsilon > 4$), the lattice parameter values a and c remain constant within the experimental error. Hence, the unit cell of the ferrite transforms from the bcc structure into the body centred tetragonal (bct) structure.

The change of the carbon concentration that is solved inside the ferrite grains during the drawing process is closely related to the tetragonal distortion of the ferrite unit cell. Indeed, the bct structure of ferrite is stabilized in the third stage ($\varepsilon > 4$) which may be coupled to the saturation of the solute carbon concentration in the ferrite. We note also that the c/a ratio reaches a steady state in the third stage where c/a = 1.007 ± 0.002. This is an unexpected observation since the tetragonal distortion of the ferrite due to solute carbon is usually known from as-quenched Fe-C martensite with high carbon concentration. Hence, the fundamental question arises whether severe plastic deformation can produce the same type of distorted phase, i.e. a deformation-driven Fe-C martensite.

Fig. 1c shows the lattice parameters of martensite from the different studies compared with our current data. Surprisingly, the measured lattice parameters for our current material fit well with lattice parameters of martensite determined by Kurdjumov et al. [6]. An even better agreement is obtained with an extrapolation of the data of Roberts [7]. Our data extend the as-quenched martensite data reported in [6] and [7] to lower C contents indicating that wire drawing induces a martensite-like tetragonal distortion of the initial bcc Fe phase. These observations exhibit a clear signature of the ordering of carbon atoms on the octahedral interstitial sites causing the ferrite unit cell to be distorted.

The thermodynamics behind the order-disorder transformation of the Fe-C system has been formulated long ago by Khachaturyan et al. [9] using microscopic elasticity theory. This theory, when coupled with DFT [10], provides a reasonable agreement with the experimental order-disorder transition of a 'usual' as-quenched Fe-C martensite. However, the mechanically driven bcc-bct transition observed in this work cannot be explained by this previous theory. Therefore, in this work, a new model has been developed that captures the strain induced interaction of C with the host matrix and which can be extended to wire drawing conditions. The new model provides not only an excellent agreement with experimental observation for the as-quenched martensite (red line and square in Fig. 2), but captures also the effect of the applied strain — exerted by the wire drawing process — within a renormalized C formation energy. As shown in Fig. 2 by the blue line, by considering 0.4 % uni-axial strain along [100], our new theory can explain the unusual tetragonal distortion measured in the present work for the low C concentrations (blue filled circles in Fig. 2).

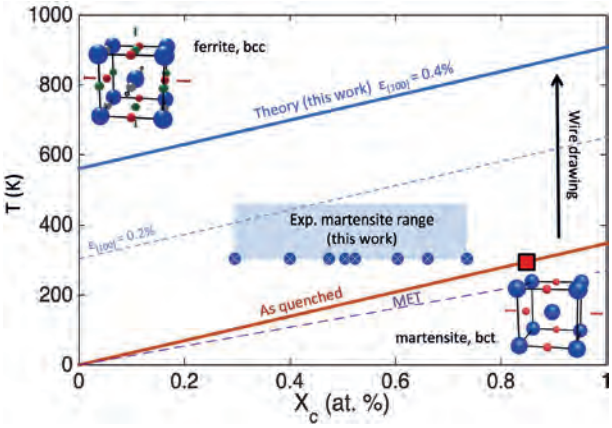

Fig. 2: *Predicted equilibrium phase diagram of Fe-C solid solutions calculated by means of DFT calculations. The order-disorder transformation temperatures are plotted as a function of carbon concentrations for the systems under an applied elastic strain of 0.4% (blue line) and also in the absence of any strain (red line). The red square corresponds to the only available experimental data point for an as-quenched martensitic transformation. The blue dots represent C concentrations of the tetragonally distorted martensite measured in this work. The dashed line represents the order-disorder transformation predicted by means of microscopy elasticity theory in Ref. [10].*

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Investigation of Hydrogen Trapping, Activity and Exposure Time on Embrittlement of High Strength Steels under Load

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Most advanced steel grades have strengths in the gigapascal range. At these strength levels, the susceptibility to hydrogen embrittlement (HE) is particularly acute. The main sources of hydrogen in steel components are the finishing or reconditioning steps used to clean or apply protective coatings, welding or annealing in hydrogen-bearing atmospheres. Another less obvious and controllable (but certainly over the life-time very important) mechanism responsible for H-uptake is atmospheric corrosion or galvanic coupling during service.

For assessment of HE usually short testing is performed by adjusting different levels of hydrogen and then performing a relatively fast mechanical test. Moreover, such tests are usually performed on some specific high alloyed steel of practical interest, while methodologically relevant screenings of a wide spectrum of materials are missing. For these selected materials, the risk of failure is typically correlated with the amount of diffusible hydrogen only. It remains an open question whether much smaller hydrogen activities, but over more extended times and with an application of permanent strain or stress, can add up to similar failure risks. Hence, the fundamental dependence of HE on the parameters time, hydrogen activity and load is not yet sufficiently investigated.

For a fundamental understanding of these parameters we follow a two-fold strategy. For the experimental approach a specially designed *in situ* setup is build. It allows us to charge the sample with hydrogen during a creep or tensile test. In parallel, *ab initio* and larger-scale tight binding calculations are performed to simulate the trapping mechanisms and kinetic processes. Systematic investigations of the above mentioned experimental parameters and their theoretical counterparts will provide a HE matrix (in particular for long times and low-H activities) and a correlation of embrittlement mechanisms with H-trap sites. We invested into design and production of *in situ* cells for long term (up to months) creep experiments, which allow us to test the matrix parameters in a methodical and statistical way.

To avoid a narrow focus on specific steel grades, we concentrate in theory and experiment on a model alloy system with a chemical composition and microstructure features that represent ferritic steels in general and give us a possibility to cover a wide range of grain sizes, dislocation densities and other H trap sites. For these purposes Fe-5%Ni model alloy is prepared in the MA. To characterize the degradation of the material creep, tensile tests and scanning electron microscopy (SEM) are used. Additionally, the trap structure before and after the *in situ* mechanical testing is analyzed with a thermal desorption spectroscopy (TDS) using a novel ultra high vacuum-based TDA-MS (thermal desorption mass spectroscopy) setup designed in the GO [1]. For a lateral resolution of H-trapping a wide spectrum of H-sensitive analytical techniques available at the GO will be used. In parallel, TDS is addressed with kinetic Monte-Carlo simulations based on the atomistic parameters determined in the CM. The challenges of the approach make this project an interdisciplinary one, where the expertise of different departments is combined to achieve an ambitious goal.

To get first experimental insights, we focus on two very different conditions of the Fe-5%Ni alloys – annealed (A) and cold rolled (CR). The samples are H-charged at different potentials *in situ* in a cell containing 0,1M NaOH while a load of 0,95 RM is

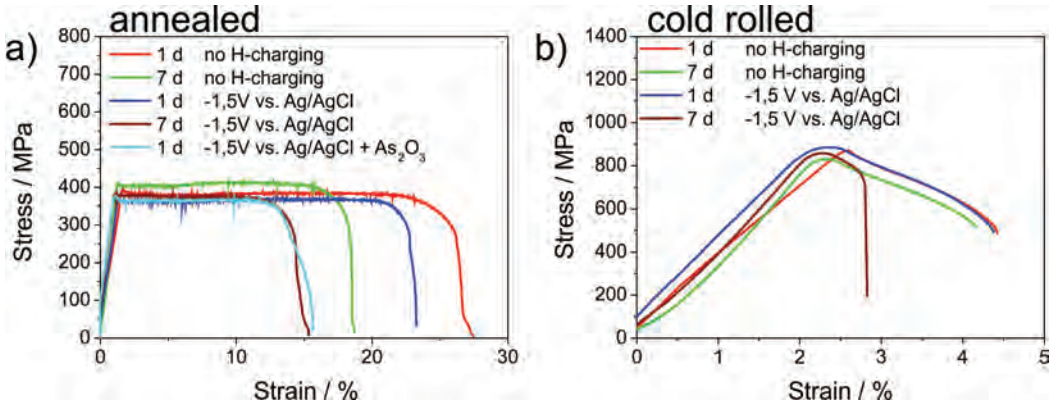

Fig. 1: *Tensile test curves for a) annealed A and b) cold rolled CR model alloy.*

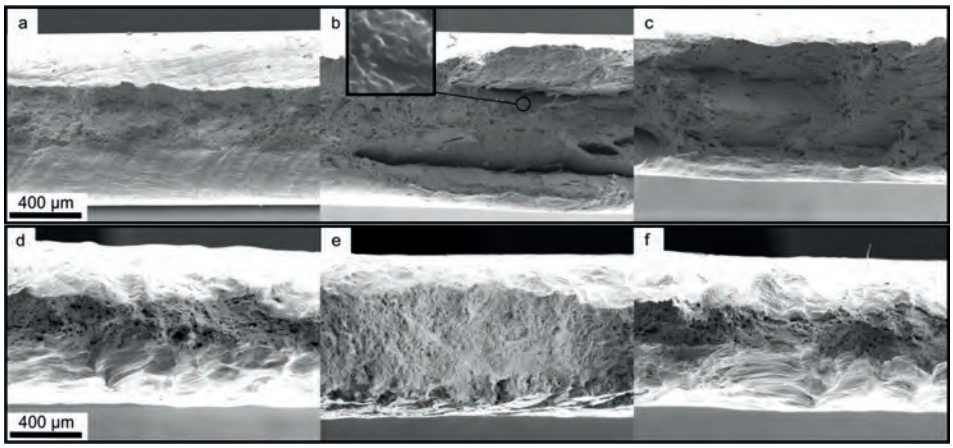

Fig. 2: *a,b,c) CR; d,e,f) A-sample. a,d) no H-charging; b,e) 24h charging + As_2O_3 and c,f) 7d charging.*

applied. During further experiments, the parameters load; potential, H-activity and time are varied to get a HE-matrix for each material state. After the creep test with varying exposure times, the sample is pulled in a tensile machine at a rate of 10^{-4} s^{-1} until fracture to get a stress-strain curve and to analyze the fracture surface. Pieces of a sample gauge length are cut and analyzed with TDS before and after the creep test.

The HE occurs in both cases after 24h during HE reference tests (with recombination inhibitor) (Fig. 1). As expected, the most drastic effect is seen in the case of CR samples, which failed completely during *in situ* creep. At the fracture surface (Fig. 2) cracks and blisters are seen in the bulk of the specimens parallel to the surface. Charging without inhibitor leads to only slight reduction in fracture deformation in A-samples after 24h, but after 7 days the degradation is clearly visible. TD- analysis of as-received A-samples showed no H-desorption peaks, for CR material 2 peaks with H-desorption activation energy of approx. 29 and 38 kJ/mol have been found (Fig. 3). After the creep under H-charging for 24h one H-desorption peak (29kJ/mol) was found also for A-material, thus this peak corresponds to hydrogen trapped at dislocations. The second peak is due to the hydrogen trapped in micro voids at inclusion-matrix interfaces inside CR material.

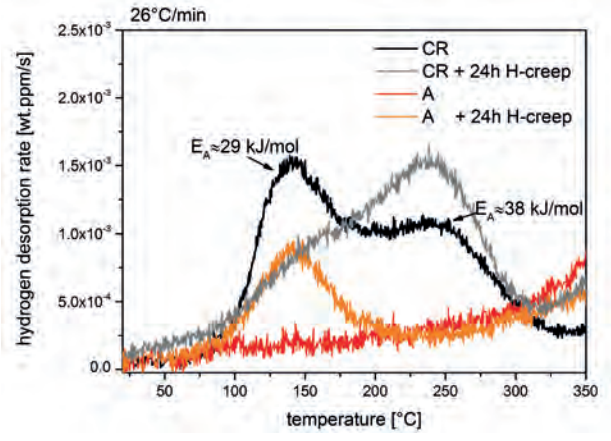

Fig. 3: *TD-spectra of A and CR model alloy before and after 24h in situ creep.*

The trapping behaviour of the most important microstructure features considered in experiment, namely grain boundaries, phase boundaries and dislocations, has been analyzed theoretically. The tendency of hydrogen to become trapped by grain boundaries in ferrite depends very sensitively on the local geometry. Parameters such as the grain boundary energy and the angle of misorientation do not appear to correlate well with the affinity of hydrogen to the boundary. However, we have found that a class of [110]-terminated twist grain boundaries is particularly attractive for hydrogen, due to substantial interstitial voids which are over-coordinated in comparison to bulk ferrite. The ferrite-cementite phase boundary is another efficient trapping site for hydrogen. The reasonably low diffusion barrier from the ferrite into the boundary layer further supports the trapping, while diffusion into or within cementite is characterized by very high barriers. The results of these simulations, such as the H-trapping energies and diffusivities in the vicinity of such features, as well as the density of H-traps within the microstructure, are used as input parameters for scale-bridging models of H-diffusion (such as kinetic Monte Carlo) currently performed in collaboration with colleagues at the Interdisciplinary Centre for Advanced Materials Simulation at the Ruhr-Universität Bochum, in order to simulate and interpret the experimentally determined TD-spectra.

The next steps will be to proceed with the experimental HE matrix. Precipitates will be introduced as further trap sites to the material. Ti and Cr carbides will be considered in experiments as well as in simulations. In order to directly link the hydrogen activity to simulations, permeation experiments [2] will be carried out, a gauge length of the tensile samples will be analyzed before and after *in situ* creeping, using techniques able to give a laterally resolved insight into a qualitative description of the H-trapping sites.

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Towards Self-Healing Metals

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The field of self-healing materials is dominated by polymers (Fig. 1) since chemical reactions in polymers are very efficient in producing a significant energy release compared to the typical bonding strength. In contrast, in ceramics and metals, diffusional processes that are needed to transport the self-healing agents to the damaged sites are slow at ambient temperatures. Despite this challenge there is an increasing interest to design self-healing metals (see black curve in the inset of Fig. 1) due to the potential economical impact. Dr. C. Tasan and Dr. B. Grabowski were recently awarded a grant within the DFG Priority Programme SPP1568 for their innovative idea of employing nano-shape memory alloy (SMA)-dispersoids as self-healing agents in metals. The joint experimental-theoretical work has recently been cumulated in a review article on self-healing metals [1].

The presently available/proposed concepts can be subdivided into two categories [1]: self-healing on the nano length scale and self-healing on the macro length scale (Fig. 2). The newly proposed concept of Tasan and Grabowski ("nanoSMA-dispersoids") falls into the first category. The aim of the concepts from the first category is to heal damage on the nanometer length scale, i.e., nano-cracks. The high-T precipitation concept (Fig. 2a) requires a microstructure with a supersaturated amount of solute atoms which exhibits precipitation in regions where nano-voids are present. The low-T precipitation concept (Fig. 2b) is closely related, but solute atoms need to segregate to dislocation cores. When localization leads to stress concentration and formation of nano-voids, the mobile solute atoms are attracted and diffuse through the dislocations towards the stress region. Precipitation within the nano-voids eventually leads to void closure and healing of the damaged region.

The second category of self-healing approaches in metals aims at healing macro-cracks. The SMA-clamp&melt concept (Fig. 2d) requires a composite microstructure with SMA reinforcement wires embedded in a solder matrix material. Under stress a crack is produced in the solder material, which triggers a transformation in the SMA phase. Self-healing is achieved by heating which leads to a contraction of the sample. Upon further heating the cracked surfaces melt and rejoin. The solder tubes/capsules concept (Fig. 2e) emulates the original self-healing concept employed in polymers: a solder material is encapsulated inside of ceramic capsules inside a host matrix of a higher melting point and ultimate tensile strength material. The solder is activated only, once a crack in the host matrix has formed, by increasing the temperature above the melting temperature of the solder. The solder then wets the crack surfaces, fills the crack, and solidifies closing the crack thereby. The coating agent concept (Fig. 2f) is a very similar approach, with the main difference being the utilization of a coating for the self-healing. The electro-healing (Fig. 2g) is achieved by immers-

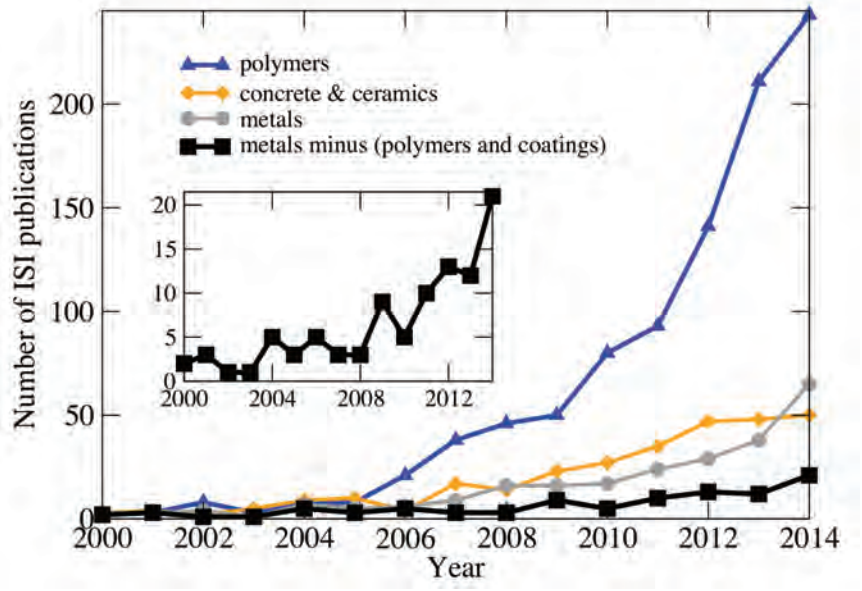

Fig. 1: *Publication numbers from ISI Web of Knowledge for the last 14 years in the field of self-healing polymers, concrete & ceramics, and metals. The inset shows a zoom-in for the black curve.*

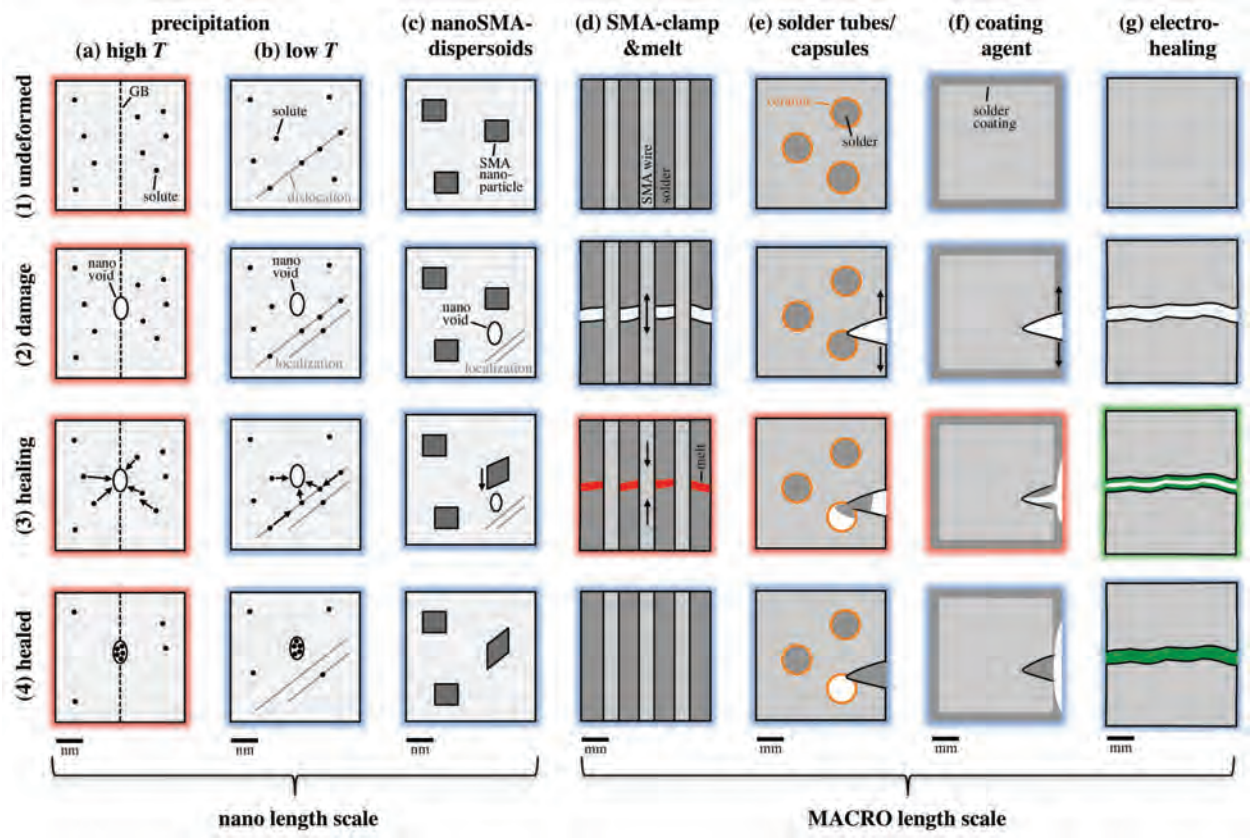

Fig. 2: *Schematic overview of the proposed/investigated self-healing concepts in metals. See main text for details.*

ing a damaged sample into an electrolyte solution and applying a voltage. The following electrochemical reaction leads to deposition of material inside the crack eventually closing it.

The nanoSMA-dispersoid concept (Fig. 2c) proposed and investigated by Tasan and Grabowski is motivated by recent atomistic simulations which clearly reveal that a stress-driven grain boundary was able to heal an approaching nano-crack. The main idea is to encapsulate the shape memory effect in nano-dispersive coherent particles which shall act as self-healing agents providing autonomous self-healing of metals. The coherent shape memory nano-particles will be introduced into and stabilized by a standard solid solution metallic matrix. The coherent host matrix will exhibit standard mechanical properties such as strength, ductility, and fracture toughness. The special and novel self-healing properties will arise by optimizing the size and distribution of the shape-memory nano-particles such as to guarantee an optimum long-term resistance to nano-cracks which - in normal circumstances -would trigger the onset of fracture. For the present purposes, nano-cracks and their stress/strain fields will act as local stress sources activating the transformation of the nanoparticles and thereby the self-healing process.

The highly challenging nature of the proposed goals calls for an integrated approach combining state of the art finite temperature *ab initio* simulations and *in situ* multiscale experimental characterization techniques in conjunction with long standing alloy design knowhow. Current focus is on a specific material system, Ti-Ni-V, with Ti-Ni as the shape memory alloy for the nano-particles. The mechanisms shall be investigated for this model system, however, the developed methodology and knowledge will apply to other materials given similar transformation properties.

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Investigations on the Local Bonding Strengths and Bonding Mechanism of Aluminium-Steel Joints Produced by Cold Forging

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Cold forging is a promising method to achieve dissimilar joining to facilitate the design of novel materials combinations. Combining materials with different physical and mechanical properties allows a large variety of applications in the manufacturing industry. For light weight construction, in particular the combination of steel and aluminium, has a significant importance, especially in automotive and aeronautics industries. Established fusion welding processes, where one or both of the materials are molten, typically lead to the often uncontrolled and rapid formation of Fe/Al intermetallic phases. Brittleness of extended Fe/Al phases results in weak bonds and poor weld quality [1, 2]. Therefore, cold welding by plastic deformation, e.g. cold forging, is an attractive manufacturing technology for future applications, with the potential to minimise or control the formation of intermetallic phases in the interfacial region [3].

Nevertheless, the mechanism of the bond formation in cold welding remains largely unexplored. According to the macroscopic model of Bay [4], breaking of cover layers, e.g. metal oxides, occurs after exceeding a critical formability. Juvenile metal extrudes between these cracks, which results in an adhesive joint formation. This macroscopic model does not consider details on an atomic scale around the interface between the partners. In addition, bond strength of joints depends on welding conditions, such as temperature, surface conditions and surface enlargement [5]. To control the formation of intermetallics, and to maximise adhesion, a more quantitative understanding of processes on an atomic scale is required.

One topic of recent investigations was to elucidate the role of primary heat treatment on the bond strength in cold forging of AA6082 aluminium alloy and C15 steel. A cross section of the resulting geometry is shown in Fig. 1. Steel itself is difficult to cold-weld, amongst other reasons because of its hardness [6]. Hardness can be modified by “soft annealing”, resulting in an alignment of the hardness of steel to the value of AA6082. This heat treatment results in the reduction of flow stress in the steel which means that soft annealed steel shows stronger bonds. According to finite element method (FEM) simulations of the cold forging process considering effects of the surface enlargement and normalized contact normal stress, the strongest bonds are expected in region (II) (Fig.1). The consequence is a stronger global bond of the joint. For determining the local bond strength, tensile specimens were cut by spark erosion from areas of interest along the joint interface (Fig. 1). A summary is shown of the resulting tensile strength of two different heating states of the C15 steel, soft annealed for 1 h (“sa”), and for 5 h (spheroidized, “s”) [6, 7].

Because of the small extrusion at position (III), this region is not contributing to the overall bond. Hence, the preparation of tensile specimens was not feasible as samples already disintegrated during the preparation. Experimental results show a weak bond in region (I), and the expected strongest bond in region (II). The softening of the C15 steel resulted in an increase of the bond strengths in regions (I) and (II). The resulting fracture after the tensile test can be divided into three major zones. In the first zone, ductile failure

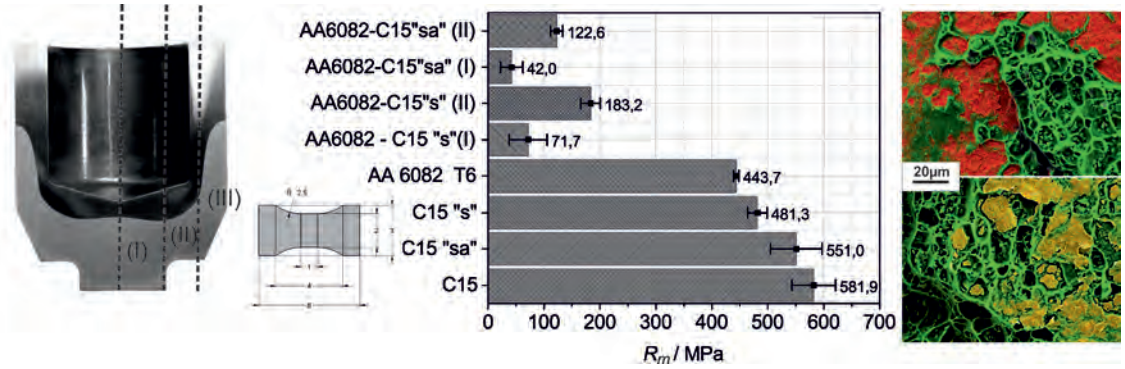

Fig. 1: *Tensile strengths of welds at different positions as indicated in the cross section through the weld geometry on the left, compared to the base materials. Right: EDX elemental maps showing Al (green) and Fe (red) of the fracture after tensile test (top=steel side, bottom=Al side).*

of the aluminium is clearly visible. In this zone, the bond between steel and aluminium is stronger than the base material. In the second zone, the aluminium parts remaining adhered to the steel side indicate brittle failure. Finally, in the third zone, brittle failure of iron is observed, whose residues remain on the aluminium side. All three zones are contributing to the bond between steel and aluminium. The resulting tensile strength of the welds is an average with different contributions [6, 7]. One particular issue which is yet unexplored is the presence of residual stresses in the resulting workpieces.

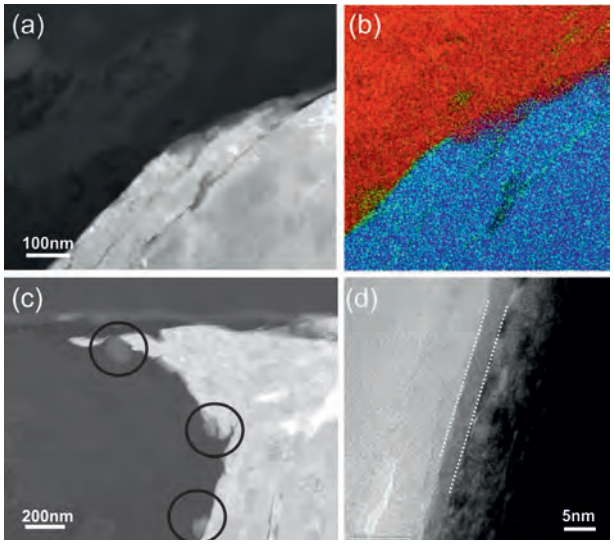

Fig. 2: *C15 steel and AA6082 welds. (a) STEM image along interface. (b) Corresponding EDX elemental map (Al – red, O – green, Fe – blue). (c) STEM image with intermetallics highlighted by black circles. (d) High resolution TEM showing a few nm thick reaction layer highlighted with white dashed lines.*

For in depth analysis of the interface after bond formation, transmission electron microscopy (TEM) was performed. A lamella for TEM experiments was extracted from region (II) via focused ion beam cutting along interface (Fig. 2). At first glance, no indication of the presence of continuous intermetallic phases is found, different from the situation during welding at high temperatures [1, 2]. However, at few spots, apparently randomly distributed along the steel/aluminium interface, intermetallics are observed (Fig. 2c). The nucleation of intermetallics may be the result of a locally increased temperature, induced by friction during plastic deformation of both partners. Whether the isolated intermetallic particles found here actually facilitate bond formation by helping to decrease interface energy and interface strain, or whether they decrease the finally observed tensile strength because they are intrinsically brittle, remains to be investigated. Crucial for the bond formation is most likely the detection of a few nm "reaction layer" along the entire interface (Fig. 2d), which consists of Fe and Al. This layer may reduce lattice strain at the interface, and its formation is most likely the key for the formation of a metallic bond between the two pieces. Further investigations are ongoing to obtain detailed information about the chemical composition and crystallography of this reaction layer.

A factor which is supposed to hinder the formation of metallic bonds is the presence of oxides at the interface [7]. In the energy-dispersive x-ray spectroscopy (EDX) elemental maps (Fig. 2b), the presence of oxygen in the interface region is obvious. Further, oxide-rich regions are found 10s of nm away from the interface. An important oxide source is the presence of oxide on the materials prior to welding. These oxides remain inside the final joint. The chemical or electrochemical removal of oxides is a promising line to increase the bond strength at the interface.

Summarising, soft annealing of steel increases the macroscopic bond strength in dissimlar welding steel and aluminium by cold forging. A maximum tensile strength of 183 MPa has been obtained for 5 h annealing (spheroidizing), still significantly below the corresponding values of the base materials. Investigations at the nanoscale showed the presence of a few nm thick reaction layer consisting of Fe and Al along the entire interface, which may be crucial for bond formation.

This work was conducted in the Priority Programmeme "Joining by Forming" (SPP1640) of the German Research Foundation (DFG).

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Structural Degradation of Fuel Cell and Electrolyzer Catalysts

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The ever-improving synthesis techniques have propelled the field of material science towards the design of an increasingly broader variety of catalytic structures, spanning from elaborated support architectures to complex nano-engineered catalytic structures. Nonetheless, with the advances in activity performances the careful consideration of the durability of such structures has too often been overlooked. Paramount for the viability of an electrocatalyst for industrial application is its ability to conserve the initial performances during the operative life of the device. In several energy-conversion applications the conditions found at the electrode are fairly aggressive and often induce a complex interplay of different degradation pathways [1-5]. Thus, the catalyst is bound to undergo a series of morphological and compositional modifications necessarily affecting its electrochemical performances.

To effectively suppress, or at least thwart, the overall performance decay, it is crucial to first identify and understand the individual contributions, which together lead to the structural degradation of the electrode materials. Mirroring the complexity of such (electro-) chemical processes, a thorough investigation of this crucial issue requires the use of a variety of experimental tools [2, 6]. In our electrocatalysis research group (GO), the back-bone of general investigation strategy consists of the coupling of macroscopic electrochemical characterization techniques (e.g. Rotating Disk Electrode, Scanning Flow Cell) and microscopic transmission electron microscopy. Thus, the combination of these two different research backgrounds stemming from the active collaboration of the GO, and the NG is instrumental to understand the correlation between the decay in electrochemical performances and the structural modifications at the nanoscale.

To date, the implementation of this strategy has been proven highly successful in resolving the complex convolution of degradation pathways affecting both state-of-the-art Pt catalysts [1] and advances catalytic systems, e.g. porous nanostructures [2]. Furthermore, the deep fundamental understanding of the processes acting at the nanoscale allowed the development of durability-tailored nanocatalysts, introducing the concept of confined alloying and, de facto, opening the way for new-generation catalytic systems [6].

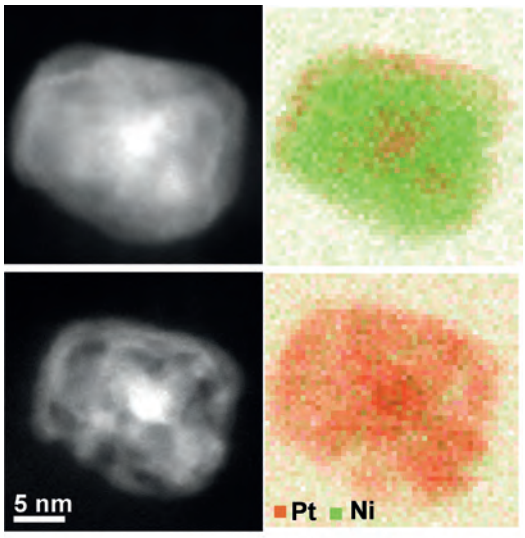

Fig. 1: *Comparison of High Angle Annular Dark Field images (HAADF) and Electron Energy Loss Spectroscopy scans (EELS) before and after electrochemical treatment. The direct observation of the catalyst allows following the compositional and morphological changes happening at the nanoscale.*

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PART IV.

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Yuki Toji, M.Sc. (Japan), JFE Steel Corp. Fukuyama/JP; Jul 2011 to Jun 2013

Dr. Bernhard Völker (Austria), KAI Kompetenzzentrum Automobil- u. Industrieelektronik GmbH/AT; Oct 2012 to Sep 2014

Dr. Marton Vörös (USA), Argonne National Laboratory/US; Feb 2014 to Dec 2015

Dr. Alexander Wimmer (Austria), KAI Kompetenzzentrum Automobil- u. Industrieelektronik GmbH, Villach, Nov 2012 to Nov 2014

Prof. Jim Wittig (USA), Vanderbilt University/US; funded by DFG SFB 761 ‚Stahl *ab initio*'; Jul to Aug 2014; Jul to Aug 2015

Yinghua Xin (China), Central South University/CN; Sep 2015 to Sep 2016

Dr. Lei Yang (China), State Key Lab of Crystal Materials/CN; May 2014 to Apr 2015

Olgun Yilmaz (Turkey), Middle East Technical University/TR, Erasmus scholarship; Jun to Sep 2014

Suhyun Yoo (South Korea), RESOLV/DE; Mar 2015 to Oct 2016

Jiecen Zhang, M.Sc. (China), Northeastern University/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2016

Huan Zhao, M.Sc. (China), Chongqing University, Chongqing; China Scholarship Council (CSC); Oct 2014 to Sep 2019

Tianyi Zhou (UK), University of Cambridge/UK, Jul to Aug 2014

Rachel Zucker (USA), Massachusetts Institute of Technology (MIT)/US; Apr to Jun 2014 & Feb to Apr 2015

Scientific Honours

2013

Fady Archie won the Science Slam “FameLab NRW”, Mar 2013

Jennifer Baseler received the Apprentice Prize of the IHK Düsseldorf, Oct 2013

The Gesellschaft für Materialographie Rhein-Ruhr gmr², established by *Angelika Bobrowski* and *Heidi Bögershausen,* was awarded the Metallographie-Preis 2013 of the DGM, Friedrichshafen (Germany), Sep 2013

Heidi Bögershausen, Herbert Faul and *Achim Kuhl* received honours from the IHK Düsseldorf for outstanding achievements in personal training, Nov 2013

Dr. Serhiy Cherevko received the ISE Electrochimica Acta Award, awarded in Mexico at the ISE annual meeting 2013

Dr. Oana Cojocaru-Mirédin won the Ernst-Haage Award of the Max Planck Institute for Chemical Energy Conversion (MPI-CEC, Mülheim a.d. Ruhr), Dec 2013

Prof. Gerhard Dehm became a member of the Board of Governors of Acta Materialia, Inc, May 2013

Prof. Gerhard Dehm obtained the Controlled Substance Award for Conferee Most Addicted to ECI Conferences at Composites at Lake Louise 2013, Alberta (Canada), Nov 2013

Dr. Martin Friák received the Poster Award 1st price at the the Euro BioMat 2013 conference in Weimar, Germany, Apr 2013

Peter J. Imrich obtained a Best Poster Award at the ECI 2013 conference in Olhao (Portugal), Oct 2013

Dr. Ioannis Katsounaros received an outgoing Marie-Curie Fellowship for a research stay at the Argonne National Laboratory, US, and the Leiden University, NL, for a total of 3 years (2013)

Dr. Björn Lange received the Otto-Hahn Medal of the Max Planck Society in Jun 2013

Dr. Duancheng Ma won the Borchers Plakette of the RWTH Aachen, Jun 2013

Vera Marx obtained a Best Poster Award at the ECI 2013 conference in Olhao (Portugal), Oct 2013

Dr. Karl Mayrhofer received the Science Award Electrochemistry 2013 sponsored by BASF and VW

Paul Neddermann received the Springorum-Denkmünze, Jul 2013

Jens Nellessen received the Springorum-Denkmünze, Jul 2013

Bastian Philippi obtained a Best Poster Award 1st Prize at the GDRi CNRS Mecano General Meeting in Düsseldorf (Germany), Jul 2013

Dr. Anna Schuppert participated in the 63rd Lindau Nobel Laureate Meetings in Jun 2013

Dr. Mira Todorova received the Best Poster Award of the Calphad Conference in San Sebastian, May 2013

Dr. Angel Topalov received the Förderpreis der GDCH for the best work in electrochemistry of a junior researcher in 2013

2014

Dr. Theodoros Baimpos received the IUMRS-ICYRAM 2014 Poster Award in Oct 2014

Dr. Poulumi Dey received a Best Poster Award at the Asia-Sweden meeting on understanding functional materials from lattice dynamics conference, Indian Institute of Technology Guwahati, India, Jan 2014

Dr. Blazej Grabowski got an ERC Starting Grant of the European Research Council (European Union’s Horizon 2020 research and innovation programme (grant agreement No 639211) in 2014

Jan-Philipp Grote received the Springer/Hysa Poster Award in Oct 2014

Dr. Wei Guo received a best poster award at the MRS Fall Conference, Dec 2014

Dr. Wei Guo received the „2014 Chinese Government Award for Outstanding Self-financed Students Abroad“, 2014

Dr. Nejc Hodnik got a Marie-Curie Intra-European Fellowship „EIWBinsTEM— Development of electrochemical water based in-situ TEM and study of platinum based nanoparticles potential- and time-dependent changes“, Apr 2014

Qingyun Hu received a IUMRS-ICYRAM 2014 Poster Award in Oct 2014

Minjie Lai received the best student poster on the 3rd International Workshop on Physics-Based Modelling of Material Properties and Experimental Observations with special focus on Plasticity and Creep, Jun 2014

Dr. Karl Mayrhofer won the Dechema-Preis der Max-Buchner-Forschungsstiftung, Nov 2014

Dr. Josef Meier received the „Förderpreis der GDCh-Fachgruppe Nachhaltige Chemie“, Sept 2014

Georgios Polymeros received the Ballard CSC (Canadian Society of Chemistry) Poster Prize 2014

Prof. Dr.-Ing. Dierk Raabe became member of the „Akademie der Wissenschaften Leopoldina“ (Sektion 27, Technikwissenschaften), Mar 2014

Prof. Dr.-Ing. Dierk Raabe became Facultaire Honorary Professor at Katholieke Universiteit Leuven (KU Leuven), Department of Materials Engineering, Nov 2014

Prof. Dr.-Ing. Dierk Raabe renewed his membership of the German Council of Science and Humanities (Wissenschaftsrat), 2014-2016

Dr. Anna Schuppert won an outgoing post-doc research fellowship of the French Embassy 2014

Torsten Schwarz received the E-MRS Graduate Student Award, May 2014

Dr. Pratheek Shanthraj got an AICES postdoctoral fellowship starting in Jul 2014

Halil Sözen received a Merkle Scholarship for “First principles calculations for complex magnetic materials”, Sep 2014

Dr. Frank Stein became a member of the editorial board of the journal Intermetallics, Jan 2014

Thomas Utzig received the CAI-STEM SFA 2014 Poster Award in Aug 2014

Dr. Markus Valtiner got the „Max-Buchner-Forschungsstipendium“ starting in Jul 2014

Ashokanand Vimalanandan won the Young Author’s EFC Poster Prize in Oct 2014

Dr. Alexander Wimmer received the Award of Excellence from the Austrian Federal Ministry of Science, Vienna (Austria), Dec 2014

Dr. Stefan Wippermann is one of the winners of the BMBF NanoMatFutur competition setting a group on “Semiconducting nanocomposites with tailored optical and electronic properties” in Jan 2014

Dr. Claudio Zambaldi won a poster award at the 17th International Conference on Textures of Materials ICOTOM, Aug 2014

2015

Dr. Pascal Beese participated in the 65th Lindau Nobel Laureate Meetings in Jun 2015

Dr. Pascal Beese won the Leopoldina Preis für junge Wissenschaftler, Nov 2015

Dr. Pascal Beese got the „Deutscher Studienpreis – Körber Stiftung“, Nov 2015

Christian Broß won the best poster prize at the Mikpräp Fachtagung 2015

Christian Broß won the Apprentice Prize of the Max Planck Society, Jul 2015

Su-Ting Cheng received a Best Poster Award at the Faraday Discussions Corrosion Chemistry Meeting of the Royal Society of Chemistry, Apr 2015

Dr. Peter J. Imrich’s talk at the Nanobrücken 2015 workshop was awarded as ‘Best Student Talk’, Potsdam, Apr 2015

Dr. Christoph Kirchlechner became member of the Beamtime Review Panel of the BESSY synchrotron source, Oct 2015

Dr. Fritz Körmann received a DFG Research Fellowship “Ab-initio-Studie zu High Entropy Alloys: Grundzustands- und darüber hinausgehende Eigenschaften“, May 2015

Dr. Sergiy Merzlikin received a Paper Award in Metallurgical Research and Technology “Prove of hydrogen formation through direct potential measurements in the rolling slit during cold rolling”, Apr 2015

Dr. Alena Michalcová received the “1st Place according to expert public – vox populi” in the Competition “The most beautiful colour or black-and-white micrograph of non-ferrous metals” at the Aluminum and non-ferrous Metals 2015 Conference, Bystrice nad Pernstejnem, Czech Republic, Oct 2015

Dr. Alena Michalcová received the “3rd Place according to expert committee” in the Competition “The most beautiful colour or black-and-white micrograph of non-ferrous metals” at the Aluminum and non-ferrous Metals 2015 Conference, Bystrice nad Pernstejnem, Czech Republic, Oct 2015

Lutz Morsdorf got a Postdoctoral Fellowship for North American and European Researchers from (JSPS), Feb 2015

Nicolas Peter received the ‘Best Talk Award - 3rd Place’ at the INASCON, Basel (Switzerland), Aug 2015

Jiali Zhang received the 3rd best Poster Award at the GDRI CNRS Mecano General Meeting at MPIE, Jul 2015

Participation in Research Programmes

National:

BMBF

„Combinatorial electrocatalytic CO2 reduction (ECCO2)“, BMBF - „Technologies for Sustainability and Climate Protection“, Oct 2011 - Sep 2016

„MANGANESE – mechanistic investigations of model and applied electrodes for the oxygen evolution.“, BMBF, May 2015 – Apr 2019

„NeKat – New electrocatalysts for application in automotive fuel cell stacks“, BMBF, Nov 2011 – Nov 2014

„Novel corrosion protection coatings compatible with hot forming (KoWUB)“, BMBF, May 2012 – Apr 2015

„Optimizing solar cell efficiency based on 3-dimensinal chemical analysis on the atomistic scale (Optimierung des Wirkungsgrades von Solarzellen basierend auf 3-dimensionalen chemischen Analysen auf atomarer Skala)“, BMBF NanoMatFutur, Feb 2013 – Jan 2017

„RADIKAL - Resource-saving material substitution by additive & intelligent FeAl material concepts adapted for light and functional building“, BMBF MatRessource, Feb 2013 – Jan 2016

„RAVE-K - Ressource friendly design for precious metal containing switch materials for low voltage applications“, BMBF MatRessource, Jun 2013 – May 2016

“Semiconducting nanocomposites with tailored optical and electronic properties (NanoSolar)”, BMBF NanoMatFutur, Jan 2014 – Dec 2017

BMWi

„Development of novel high temperature proton exchange membrane (HTPEM) fuel cells with improved degradation behavior“, Zentrales Innovationsprogramm Mittelstand – ZIM, BMWi, Jan 2015 – Nov 2017

DFG

DFG Priority Programmes & Collaborative Research Centres

„*Ab initio* study on the coupling of lattice and magnetic degrees of freedom and the role of interfaces in magneto-caloric materials“, DFG Priority Programme - SPP1599: Caloric effects in ferroic materials: New concepts for cooling, Oct 2012 – Dec 2016

„Design and Generic Principles of Self-Healing Materials“, DFG SPP 1568, May 2014 – Dec 2017

„From Atoms to Turbine Blades – a Scientific Approach for Developing the Next Generation of Single Crystal Superalloys“, DFG SFB/Transregio 103, Jan 2012 – Dec 2015

„Heapocrates: Healing Polymers for preventing Corrosion of Metallic Systems“, DFG Priority Programme - SPP 1568: Design and Generic Principles of Self-Healing Materials, May 2011 – Apr 2014

„Investigation and enhancement on bonding by cold bulk metal forming processes“, DFG Priority Programme - SPP 1640: Joining by Plastic Deformation, Nov 2012 – Dec 2015

„Quantum mechanically guided design of ultra strong glasses, DFG Priority Programme - SPP 1594: Topological Engineering of Ultra-Strong Glasses“, Jul 2012 – Dec 2016

„Mechano-chemical coupling during precipitate formation in Al-based alloys“, SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Sep 2014 – Aug 2017

“Metal oxide nanostructures for electrochemical and photoelectrochemical water splitting”, SPP 1613, Oct 2015 – Sep 2018

„Modeling bainitic transformations during press hardening“, SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Sep 2014 – Aug 2017

„Nanostructured Hierarchical Oxide Photoelectrodes for Photoelectrochemical Water-Splitting“, DFG Priority Programme - SPP 1613: Regeneratively Produced Fuels by Light Driven Water Splitting: Investigation of Involved Elementary Processes and Perspectives of Technologic Implementation, Apr 2014 – Sep 2018

„Regeneratively Produced Fuels by Light Driven Water Splitting: Investigation of Involved Elementary Processes and Perspectives of Technologic Implementation“, DFG SPP 1613, Oct 2015 – Sep 2018

„Steel - *Ab Initio*. Quantum Mechanics Guided Design of New Fe-based Materials“, DFG SFB 761, 1st period: July 2007 – June 2011, 2nd period: Jul 2011 – Jun 2015, 3rd period: Jul 2015 – Jun 2019

Projects at MPIE in frame of SFB 761:

- A 02 *Ab initio* thermodynamics und kinetics in the Fe-Mn-Al-C system, Jul 2007 – Jun 2019
- A 07 Microstructure mechanics and fundamentals of concurrent twinning and martensite formation, Jul 2007 – Jun 2019
- A 09 *Ab initio* based mesoscale simulation of hydrogen embrittlement, Jul 2011 – Jun 2019
- B 07 Synthesis and characterization of Reference Materials, Jul 2011 – Jun 2015
- C 01 Microstructure analytics, Jul 2015 – Jun 2019
- C 04 Fatigue, damage and stress corrosion cracking under cyclic loading, Jul 2007 – Jun 2019
- C 08 3D atomic analysis of the local chemical composition by atom probe tomography, Jul 2011 – Jun 2019
- C09 Deformation mechanisms and local residual stresses in the system Fe-Mn-C, Jul 2011 – Jun 2015
- C 10 Deformation behavior of multi-phase steels, Jul 2015 – Jun 2019
- T4: Wasserstoff-Karbid-Wechselwirkung Jul 2015 – Jun 2018

„Synthetic dental composite materials inspired by the hierarchical organization of shark tooth enameloid“, DFG Priority Programme - SPP 1420: Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials, Aug 2013 – Dec 2015

„Tailored Disorder – A Science- and Engineering-Based Approach to Materials Design for Advanced Photonic Applications“, DFG SPP 1839, Jul 2015 – Dec 2018

„Thermo-chemo-mechanical coupling during thermomechanical processing of microalloyed steels“, DFG Priority Programme - SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jun 2014 – Dec 2017

„Understanding the role of trigger signal spreading, release rate of suitable active agents and their transport rate for optimal healing in extrinsic self-healing materials“, DFG Priority Programme - SPP 1568: Design and Generic Principles of Self-Healing Materials, May 2014 – Jun 2017

DFG Research Grants

„*Ab initio* determination of free energies and derived properties (heat capacities, vacancies, solvus boundaries) for selected Al alloys containing Si, Mg and Cu“, DFG Research Grant, Jan 2010 – Feb 2016

„Deformation via the Transformation of Hierarchial Microstructures“, DfG Research Grant, Apr 2014 – Jun 2014

„Fine-scaled lamellar Fe-Al *in situ* composites: Microstructure and mechanical properties“, DFG Research Grant, Jan 2013 – Dec 2015

„Identification and overcoming of loss mechanisms in nanostructured hybrid solar cells - pathways towards more efficient devices.“, DFG, Apr – Dec 2014

„Materials World Network: Fundamentals of Peptide Materials - Experimental and Simulation Probes“, DFG - NSF Materials World Network, Jan 2014 – Dec 2016

„Mechanisms of self and impurity diffusion in Fe-Al intermetallic compounds“, DFG research Grant, Sep 2010 – Mar 2015

„Microbiological corrosion induced by highly aggressive sulphate-reducing-bacteria“, DFG, SRB, Oct 2011 – Jul 2015

„Study of grain-boundary-dislocation interactions by advanced *in situ* µLaue diffraction“, DFG Research Grant, Jan 2015 – Dec 2017

„The effective pH at the solid-liquid interface and the local ion distribution during complex electrochemical reactions“, DFG Research Grant, Jan 2014 – Aug 2015

„Understanding Grain Boundary Migration - Theory Meets Experiment“, DFG Support for Scientific Meeting, Jan – Dec 2015

„Understanding the role of dislocation distribution(s) on the slip transfer across twin-boundaries“, DfG, Aug 2015 - Dec 2016

DFG Cluster of Excellence

„Electrochemistry on „dry surfaces“: electrode potential and structural order in nanoscopic electrolyte layers“, “, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Aug 2013 – Jan 2015

„Probing the molecular structure of extended solvated surfaces and interfaces“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Mar 2014 – Feb 2017

„Vibrational spectroscopy of solvent during electrode polarisation and electrochemical reactions on germanium electrodes with and without metal films“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Oct 2013 – Mar 2015.

„Zinc oxide – water interfaces: interaction-driven structural evolution“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Feb 2015 – Jul 2016

Max Planck Society

„Active coatings for corrosion protection- Aktive Schichten für den Korrosionsschutz (ASKORR)“ – MPG – FhG cooperation, May 2010 – Apr 2013

„Advanced Alloy and Process Design for laser Additive Manufacturing of Metals“, “, MPG - FhG cooperation, Apr 2015 – Mar 2018

„Early detection of material wear in high-precision machine tools – Initial wear“, MPG - FhG cooperation, Jan 2014 – Dec 2016

„International Max Research School (IMPRS) for Surface and Interface Engineering in Advanced Materials (SurMat)“, Max Planck Society, Jan 2010 – Dec 2015

MaxNet Energy, Research Cooperation, Max Planck Society, Jan 2014 – Dec 2018

State of North Rhine-Westphalia

„High-pressure Fe–Al steam turbine blade - Development of a processing route for fabrication of a highpressure iron aluminide steam turbine blade“, progress.nrw, Aug 2012 – Sep 2015

International:

Christian Doppler Society

Christian Doppler Laboratory “Diffusion and segregation mechanisms during production of high strength steel sheet” (original title: “Diffusions- und Segregationsvorgänge bei der Produktion hochfesten Stahlbands“) Jan 2008 – Dec 2014

European Union

European Research Council

„Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys (SMARTMET)“, ERC Co-Investigator Grant of the European Research Council, FP7, Feb 2012 – Jan 2017

„Time-scale bridging potentials for realistic molecular dynamics simulations-TIME-BRIDGE“, ERC Starting Grant of the European Research Council, Horizon 2020, Jul 2015 – Jun 2020

Marie Curie Actions

„Development of electrochemical water based in-situ TEM and study of platinium based nanoparticles potential- and time-dependent changes (ElWBinsTEM)“, Marie Curie Intra European Fellowship (FP7), Apr 13 – Mar 2016

„Soft Matter at Aqueous Interfaces (SOMATAI)“, Marie Curie Initial Training Network (FP7), Oct 2012 – Sep 2016

Collaborative Projects (FP7 and Horizon 2020)

„Accelerated Metallurgy - the accelerated discovery of alloy formulations using combinatorial principles (AccMet)“, Collaborative project, FP7, Jun 2014 – Jun 2016

„AlGaInN materials on semi-polar templates for yellow emission in solid state lighting applications (ALIGHT)“, Collaborative Project, FP7, Jun 2012 – May 2015

„Enhanced Power Pilot Line – EPPL“, ENIAC Joint Undertaking, FP7, May 2013 – Mar 2016

„Enhanced substrates and GaN pilot lines enabling compact power applications – PowerBase“, The ECSEL Joint Undertaking, FP7, May 2015 – Apr 2018

„Fuel Flexible, Near -Zero Emissions, Adaptive Performance Marine Engine – HERCULES 2“, Horizon 2020, May 2015 – Apr 2018

RFCS

„Advanced zinc-based hot dip coatings for the automotive application“, RFCS, Sep 2009 – Feb 2013

„Guidelines for use of welded stainless steel in corrosive environments (JOINOX)“, RFCS, Sep 2012 – Feb 2016

„High Emissivity Annealing Technique“, RFCS, Jul 2010 – Dec 2013

„Improvings teel product durability through alloy coating microstructure (MicroCorr)“, RFCS, Sep 2015 – Feb 2019

„New approaches to quantitative Hydrogen Analysis of coated steel products“, RFCS, Jul 2010 – Feb 2014

„New developments and optimisation of high strength boron treated steels through the application of advanced boron monitoring techniques (OPTIBOS)“, RFCS, Jul 2012 – Dec 2015

„New Metallurgical Tools for optimum design of modern Ultra High Strength Low Carbon Martensitic Steels (TOOLMART)“, RFCS, Jul 2013 – Dec 2016

„Screening of tough lightweight Fe-Mn-Al-C, steels using high throughput methodologies (LIGHTOUGH)“, RFCS, Jul 2015 – Dec 2018

Foundation Materials Innovation Institute

„Development of full field gradient plasticity FEM code to predict constitutive material model for dual phase steels“, Jan 2011 – Dec 2015

„The influence of grain and interphase boundaries on strength and fracture toughness of AHSS steels - experimental investigation on the relation between character of individual grain boundaries and grain boundary networks and their deformation behaviour“, Jul 2014 – Jun 2018

European Space Agency (ESA)

„On Beryllium Alloy & Composite Development for Space and Non-Space Application“, Jan 2014 – Dec 2016

Sino-German Center for Research Promotion (SGC)

"Liquidus surfaces and reaction schemes of the ternary systems Cr-Al-Nb and Fe-Al-Nb: Experiments and thermodynamic modelling", Chinesisch-Deutsches Zentrum für Wissenschaftsförderung, Jan 2012 – Dec 2012

Massachusetts Institute of Technology International Science and Technology Initiatives (MISTI)

"Collaborative Improvement of Photoelectrochemical Cells: Experiments and Modeling of Inexpensive Hematite Photoanode Nanostructures"

MCL – COMET K2 Program (Materials Center Leoben)

"Life time of functional multilayer ceramic systems", Materials Center Leoben, Austria, Aug 2013 - Sep 2014

Collaboration with National and International Research Institutes

National:

ACCESS e.V. Aachen, Aachen

Deutsches Zentrum für Luft- und Raumfahrt (DLR), Bonn

Forschungszentrum Jülich GmbH: Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons, Jülich

Forschungszentrum Jülich GmbH: Institute of Complex Systems Soft Condensed Matter (ICS-3), Jülich

Forschungszentrum Jülich GmbH: Peter-Grünberg-Institut, Jülich

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für allgemeine Werkstoffeigenschaften, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Feststoff- und Grenzflächen-verfahrenstechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Korrosion und Oberflächentechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Kunststofftechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Werkstoffkunde und Technologie der Metalle, Erlangen

Fraunhofer Institut für Angewandte Polymerforschung (IAP), Potsdam

Fraunhofer-Institut für Keramische Technologien und Systeme (IKTS), Dresden

Fraunhofer-Institut für Lasertechnik (ILT), Aachen

Fraunhofer-Institut für Produktionstechnologie (IPT), Aachen

Fraunhofer Institut für Silicatforschung (ISC), Würzburg

Fraunhofer-Institut für Werkstoffmechanik (IWM), Freiburg

Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Dresden

Friedrich-Schiller-Universität Jena, Otto-Schott-Institut für Materialforschung (OSIM), Jena

Heinrich-Heine-Universität Düsseldorf: Lehrstuhl für Festkörperphysik, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Lehrstuhl für organische Chemie, Düsseldorf

Helmholtz-Zentrum Geesthacht – Zentrum für Material- und Küstenforschung, Geesthacht

Humboldt Universität zu Berlin: Institut für Mathematik, Berlin

IWT - Stiftung Institut für Werkstofftechnik, Bremen

Jacobs University Bremen, Privatuniversität, Bremen

Karlsruher Institut für Technologie (KIT): Institut für Angewandte Materialien – Werkstoffkunde (IAM), Karlsruhe

Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund

Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden: Institut für komplexe Materialien, Dresden

Leibniz Universität Hannover: Institut für Festkörperphysik, Hannover

Ludwig-Maximilians-Universität München: Fakultät für Chemie und Pharmazie, München

Martin-Luther-Universität Halle-Wittenberg: Institut für Chemie, Halle

Max-Planck-Institut für Chemische Energiekonversion, Mülheim a. d. Ruhr

Max-Planck-Institut für Innovation und Wettbewerb, München

Max-Planck-Institut für Kohlenforschung, Mülheim a. d. Ruhr

Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam-Golm

Max-Planck-Institut für Polymerforschung, Mainz

Otto-von-Guericke-Universität Magdeburg, Magdeburg

Ruhr-Universität Bochum: Institut für Werkstoffe, Bochum

Ruhr Universität Bochum, Institut für Werkstofftechnik, Bochum

Ruhr-Universität Bochum: Lehrstuhl für allgemeine Mechanik, Bochum

Ruhr-Universität Bochum: Lehrstuhl für angewandte Festkörperphysik, Bochum

Ruhr-Universität Bochum: Lehrstuhl für anorganische Chemie II, Bochum

Ruhr-Universität Bochum: Lehrstuhl für Informatik im Bauwesen, Bochum

Ruhr-Universität Bochum: Institute for Experimental Physics IV - Solid State Physics, Bochum

Ruhr Universität Bochum: Institut für Geologie, Mineralogie und Geophysik, Bochum

Ruhr-Universität Bochum: Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Bochum

Ruhr-Universität Bochum: Lehrstuhl für physikalische Chemie I, Bochum

Ruhr-Universität Bochum: Lehrstuhl für physikalische Chemie II, Bochum

Ruhr-Universität Bochum: Lehrstuhl für technische Chemie, Bochum

Ruhr-Universität Bochum: Lehrstuhl für Werkstoffe der Mikrotechnik, Bochum

Ruhr-Universität Bochum: Lehrstuhl für Werkstoffwissenschaft, Bochum

Ruhr-Universität Bochum: Zentrum für Elektrochemie, Bochum

RWTH Aachen: Institut für allgemeine Mechanik, Aachen

RWTH Aachen: Institut für Eisenhüttenkunde (IEHK), Aachen

RWTH Aachen: Institut für Werkstoffanwendungen im Maschinenbau (IWM), Aachen

RWTH Aachen: Institut für Anorganische Chemie, Aachen

RWTH Aachen: Lehrstuhl für Werkstoffchemie (MCh), Aachen

RWTH Aachen: Klinik für Zahnärztliche Prothetik und Biomaterialien, Aachen

RWTH Aachen: Institut für Strahlantriebe und Turboarbeitsmaschinen (IST), Aachen

Universität des Saarlandes: Lehrstuhl für Funktionswerkstoffe, Saarbrücken

Universität des Saarlandes: Institut für Experimentelle Methodik der Werkstoffwissenschaften, Saarbrücken

Technische Universität Bergakademie Freiberg, Freiberg

Technische Universität Berlin: Institut für Chemie, Berlin

Technische Universität Berlin: Lehrstuhl für Wirtschafts-, Unternehmens- und Technikrecht, Berlin

Technische Universität Clausthal: Institut für Metallurgie, Clausthal

Technische Universität Darmstadt: Fachgebiet Datenverarbeitung in der Konstruktion, Darmstadt

Technische Universität Darmstadt: Institut für Produktionstechnik und Umformmaschinen - PtU, Darmstadt

Technische Universität Dresden, Dresden

Technische Universität Kaiserslautern: Fachbereich Physik, Kaiserslautern

Technische Universität München: Friedrich-Schiedel-Lehrstuhl für Wissenschaftssoziologie, München

Technische Universität München: Lehrstuhl für biogene Polymere, München

Technische Universität München: Lehrstuhl für effiziente Algorithmen, München

Technische Universität München: Munich Center for Technology in Society, München

Universität Bayreuth, Bayreuth

Universität Bielefeld: Fakultät für Physik, Bielefeld

Universität Bielefeld: Fakultät für Soziologie, Bielefeld

Universität Duisburg-Essen: Fakultät für Mathematik, Duisburg

Universität Duisburg-Essen: Fakultät für Physik, Duisburg

Universität Duisburg-Essen: Institut für Mechanik, Duisburg

Universität Duisburg-Essen: Institut für physikalische und theoretische Chemie, Essen

Universität Duisburg-Essen: Institut für Verbrennung und Gasdynamik – Reaktive Fluide (IVG), Duisburg

Universität Konstanz: Fachbereich Physik, Konstanz

Universität Paderborn, Paderborn

Universität Regensburg, Regensburg

Universität Rostock: Institut für Experimentelle Chirurgie, Rostock

Universität Stuttgart: Institut für Mechanik, Stuttgart

Universität Siegen: Lehrstuhl für Numerische Mechanik, Siegen

Universität Siegen: Institut für Physik, Siegen

Universität Ulm, Ulm

Universität Würzburg: Center for Digital Fabrication, Würzburg

Westfälische Wilhelms-Universität Münster: Institut für Materialphysik, Münster

International:

Academia Sinica, Institute of Physics, Taipei, Taiwan

Academy of Sciences of the Czech Republic, Institute of Physics of Materials, Czech Republic

AGH University of Science and Technology, Krakow, Poland

Argonne National Laboratory, Argonne, USA

Brown University, Providence, USA

California Institute of Technology - Caltech, Pasadena, USA

Cardiff University, UK

CEA Saclay, France

Centre de Recherches Metallurgiques C.M.R., Belgium

Centre National de la Recherche Scientifique CNRS: Centre de Recherche en Matière Condensée et Nanosciences (CRMCN), Marseille, France

Centro Tecnológico CEIT-IK, Spain

Charles University, Prague, Czech Republic

Chinese Academy of Sciences: Shanghai Institute of Optics and Fine Mechanics, Shanghai, China

Christian Michelsen Research AS, Bergen, Norway

CTM Centre Tecnològic, Manresa, Spain

Ecole polytechnique fédérale de Lausanne: Interdisciplinary Center for Electron Microscopy, Lausanne, France

Deakin University, Australia

Delft University of Technology: Faculty of Aerospace Engineering, The Netherlands

Delft University of Technology: Faculty of Applied Sciences, FAME group, The Netherlands

Eidgenössische Technische Hochschule Zürich (ETH), Zurich, Switzerland

Eindhoven University of Technology

EMPA Thun, Switzerland

Erich Schmid Institut für Materialwissenschaft, Leoben, Austria

European Space Agency ESA/ESTEC, Noordwijk, The Netherlands

European Synchrotron Radiation Facility (ESRF), Grenoble, France

German University in Cairo, Egypt

Guangxi University, Nanning, China

Hasselt University, Hasselt, Belgium

Hokkaido University of Science, Sapporo, Japan

IMDEA Materials Institute, Madrid Spain

Imperial College London: Department of Materials, Thomas Young Centre, UK

Imperial College London: Department of Physics, UK

INAC, CEA Grenoble, France

Indian Institute of Technology Guwahati: Department of Physics, India

Indian School of Mines, Dhanbad, India

Institute of Quantum materials Science, Yekaterinburg, Russia

Iowa State University, USA

Iwate University, Japan

JFE Steel Co. Steel: Research Laboratory, Japan

Katholieke Universiteit Leuven, Leuven, Belgium

KTH Royal Institute of Technology: Department of Materials Science and Engineering, Stockholm, Sweden

Kyushu University, Japan

Lawrence Livermore National Laboratory, Livermore, USA

Linköping University: Department of Physics and Measurement Technology (IFM), Sweden

Los Alamos National Lab, NM, USA

Massachusetts Institute of Technology (MIT): Department of Material Science and Engineering, Cambridge MA, USA

Michigan State University, USA

Montanuniversität Leoben: Department of Physical Metallurgy and Materials Testing, Leoben, Austria

Montanuniversität Leoben: Department of Material Physics, Leoben, Austria

Montanuniversität Leoben: Institute for Mechanics, Leoben, Austria

National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, USA

National Institute for Materials Science (NIMS), Japan

National Institute of Chemistry, Ljubljana, Slovenia

National Research Council of Italy, National Institute of Optics, Pisa, Italy

National Research Tomsk State University, Russia

NIZO Food Research, Ede, The Netherlands

Northeastern University: Physics Department and Center for Interdisciplinary Research on Complex Systems, Boston, USA

Norwegian University of Science and Technology (NTNU): Faculty of Engineering Science and Technology (IVT), Department of Engineering Design and Materials (IPM), Nano- and micro characterization of Materials, Norway

Oak-Ridge National Laboratory (ORNL): Center for Defect Physics, USA

Ohio State University, USA

Pohang University of Science and Technology, Pohang, South Korea

Pohang University of Science and Technology: Department of Materials Science and Engineering, Pohang, South Korea

Seoul National University, Seoul, South Korea

Silesian University of Technology, Gliwice, Poland

Strategisch Initiatief Materialen (SIM), Belgium

Swansea University, UK

Swerea KIMAB, Kista, Sweden

Technical University of Liberec, Czech Republic

Technical University of Denmark (DTU), Lyngby, Denmark

Technion - Israel Institute of Technology: Department of Materials Engineering, Haifa, Israel

Technische Universität Wien: Institute of Materials Science and Technology, Vienna, Austria

Technische Universität Wien: Institute of Lightweight Design and Structural Biomechanics (ILSB), Vienna, Austria

Texas A&M University: Department of Aerospace Engineering, USA

Tezpur University, Tezpur, India

United Kingdom Atomic Energy Authority, UK

Università degli Studi di Torino (UNITO), Italy

Universités d'Aix-Marseille: Institut Matériaux Microélectronique Nanosciences de Provence (IM2NP), Marseille, France

University of Amsterdam (UvA), Amsterdam, The Netherlands

University of Applied Sciences Upper Austria, Austria

University of Copenhagen: Niels Bohr Institute, Center for Quantum Devices, Copenhagen, Denmark

University of Bern, Switzerland

University of Birmingham, UK

University of California, Berkeley: Department of Materials Science and Engineering, USA

University of California, Davis, USA

University of California, Santa Barbara, USA

University of Cambridge, UK

University of Chicago, USA

University of Groningen, The Netherlands

University of Luxembourg, Luxembourg

University of Tennessee: Department Material Science and Engineering, Knoxville, USA

University of Poitiers, Institut Pprime, Poitiers, France

University of Pretoria, South Africa

University of Rouen, France

University of Science and Technology, Beijing, China

University of Sheffield, UK

University of Sydney, Australia

University of Washington, Seattle, USA

University of Zurich, Switzerland

Uppsala University: Department of Physics and Astronomy, Materials Theory, Sweden

Weizmann Institute of Science: Chemical Physics Department, Rehovot, Israel

West Virginia University, Morgantown, USA

Wigner Research Center for Physics, Budapest, Hungary

Xiamen University, Xiamen, China

Collaborating Industrial Partners and Patents

Collaborating Industrial Partners

National:

Airbus Group Innovations, München/Ottobrunn

AVANTYS engineering GmbH & Co. KG, Paderborn

BASF AG, Ludwigshafen

BASF Coatings AG, Münster

Biochem Zusatzstoffe Handels- und Produktionsges. mbH, Lohne

Bruker EAS GmbH, Hanau

Bruker Nano GmbH, Berlin

Continental Automotive GmbH, Regensburg

Daimler AG, Düsseldorf

Dr. Kochanek Entwicklungsgesellschaft, Neustadt a. d. Weinstrasse

Eickhoff Antriebstechnik GmbH, Bochum

ELCOMAX GmbH, München

ELOCORE GmbH, München

Henkel AG & Co. KGaA, Düsseldorf

Karanto Corrosion Protection Technologies GmbH, Düsseldorf

Kennametal Stellite, Koblenz

Kirchhoff Automotive, Iserlohn

Leistritz Turbinenkomponenten Remscheid GmbH, Remscheid

Nanoval GmbH & Co. KG, Berlin

Oerlikon Leybold Vacuum GmbH, Köln

OSRAM Opto Semiconductors GmbH, Regensburg

Robert Bosch GmbH, Stuttgart

Schaeffler Technologies AG & Co. KG, Herzogenaurach

Salzgitter Mannesmann Forschung GmbH, Duisburg

Sentech Instruments GmbH, Berlin

Senvion GmbH, Hamburg

Siemens AG Corporate Technology, Berlin

Thermprotec GmbH, Offenburg

ThyssenKrupp Steel Europe AG, Duisburg/Dortmund

TLS Technik GmbH & Co Spezialpulver KG, Bitterfeld-Wolfen

Umicore AG & Co. KG, Hanau-Wolfgang

Vallourec, Düsseldorf

VDM Metals, Research and Development, Werdohl

Voestalpine Böhler Welding Germany GmbH, Hamm

International:

ABB Turbo Systems AG, Baden, Switzerland

ArcelorMittal Maizières SA, Maizières-lès-Metz, France

ATI Specialty Alloys and Components, Albany, USA

Bekaert, Belgium

Centro Ricerche Fiat, Torino, Italy

GE Avio S.r.l. Avio Aero, Torino, Italy

EPCOS OHG, Deutschlandsberg, Austria

Infineon Technologies Austria AG, Villach, Austria

JFE Steel Corporation, Hiroshima, Japan

Johnson Matthey, UK

KAI Kompetenzzentrum Automobil- u. Industrieelektronik GmbH, Villach, Austria

LS Instruments AG, Fribourg, Switzerland

Molycorp Silmet AS, Estonia

Nippon Steel & Sumitomo Metal Corporation, Japan

NIZO Food Research, Ede, The Netherlands

Norsk Titanium Components AS, Oslo

OCAS NV, Belgium

Outokumpu Stainless AB, Stockholm, Sweden

Renishaw plc, UK

Rolls-Royce plc. UK

Sandvik Coromant R&D, Stockholm, Sweden

Stiftelsen SINTEF, Trondheim, Norway

Swerea KIMAB, Kista, Sweden

Tata Steel, Ijmuiden, The Netherlands

TWI Ltd., Cambridge, UK

Vallourec Research Center France, France

Voest Alpine Stahl GmbH, Linz, Austria

Wärtsilä Finland Oy, Vaasa, Finnland

Wärtsilä Netherlands B.V., Zwolle, Niederlande

Winterthur Gas & Diesel Ltd., Winterthur, Schweiz

ZF Windpower Antwerpen NV, Lommel, Belgium

Patents

Patents issued in the given time schedule

Date of Issue	Description	Inventors
June 05, 2015	**Korrosionsbeständiger austenitischer Stahl** (JP 2012519780 A)	Weber, Sebastian, Dr. Mujica Roncery, Lais, Dipl.-Ing
January 08, 2015	**Aktive Schichten für Korrosionsschutz** joint invention in context of FhG-MPG-cooperation (DE 10 2012209761.9)	Rohwerder, Michael Dr. Vimalanandan, Ashokanand Tran, The Hai Various inventors from Fraunhofer Gesellschaft Landfester, Dr. K.; Crespy, Dr. D.; Fickert, J., MPI für Polymerforschung
May 19,2009 January 01, 2013	**High carbon steel with superplasticity** (US 7.534314B2) (DE 10 2005 027 258.4)	Frommeyer, Georg, Prof. Dr. Dr. Gerick, DaimlerChrysler AG Dr. Tilmann Haug, DaimlerChrysler AG Dr. Wolfgang Kleinekathöfer, DaimlerChrysler AG
October 05, 2010 August 27, 2012 December 11, 2013 December 11, 2013	**Verfahren zum Erzeugen von Warmbändern aus Leichtbaustahl** (US 10/595,781) (KR 10-2006-7012471) (DE 50 2004 014 463.2) (EP 04802997.9)	Frommeyer, Georg, Prof. Dr. Brüx, Udo, Dipl.-Phys. Brokmeier, Klaus, Dipl.-Ing. Kroos, Joachim, Dr., Salzgitter Flaxa, Volker, Dr., Salzgitter Spitzer, K.-H., Prof. Dr., TU Clausthal

Patents filed in the given time schedule

Date of Pending	Description	Inventors
March 10, 2009 March 03, 2010	**Korrosionsbeständiger austenitischer Stahl** (10 2009 003 598.2) (PCT DE 2010/000232) (CN000102365382A) release to inventors in 10/2014 (EP 2 406 405 A1) (JP 2012519780 A) (KR 102011136840 A) (US 20120000580 A1) release to inventors in 10/2014	Weber, Sebastian, Dr. Mujica Roncery, Lais, Dipl.-Ing
December 20, 2012	**Kaltformbare, schweißgeeignete Konstruktionsstähle** (10 2012 112 703.4)	Springer, Hauke Dr.

Date of Pending	Description	Inventors
February 8, 2013 February 8, 2012	**Highly sinter-stable metal nanoparticles supported on mesoporous graphitic particles and their use** Joint invention with Studiengesellschaft Kohle mbH, transference to Studiengesellschaft Kohle mbH in January 2014 (WO 2013/117725 A1) (EP 2012 0154508)	Mayrhofer, Karl Dr. Meier, Josef Baldizzone, Claudio Schüth, Ferdi Prof.,Galeano Nunez, Diana Carolina, Bongard, Dr. Hans, MPI für Kohlenforschung
March 13, 2012	**Use of mesoporous graphite particles for electrochemical applications** Joint invention with Zentrum für Brennstoffzellentechnik ZBT GmbH and Studiengesellschaft Kohle mbH: transference to Studien-gesellschaft Kohle mbH in August 2014 (DE 10 2012 102120)	Mayrhofer, Karl Dr. Meier, Josef Peinecke, Dr. Volker, Zentrum f. Brennstoff-zelltechnik ZBT GmbH Galeano Nunez, Diana Carolina, Schüth, Ferdi Prof., MPI für Kohlenforschung
May 16, 2012	**Fabrication of nanoporous carbide membranes** Joint invention with Universitat Politecnica de Catalunya: Agreement concerning rights with UPC since 02/2013 (EP 12168207.4)	Renner, Frank Dr. Duarte-Correa, Maria Jazmin Dr. Lengsfeld, Julia Bruna, Pere Dr., BarcelonaTech
April 26, 2013	**Nanoelektroden-Partikelfalle für empfindliche spektroskopische u. elektronische Analyse** US-Patent: Appl. No. 13/872,013	Erbe, Dr. Andreas Chia-Fu Chu, Ming-Li Chu, Leonardo Lesser-Rojas, Academia Sinica Taipe

Conferences, Symposia and Meetings Organized by the Institute

2013

M. Palm organized and chaired the Intermetallics Technical Committee Meeting of the Deutsche Gesellschaft für Materialkunde (DGM) at the Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, 10 Jan 2013

H. Springer organized the workshop "Alloy Design of Advanced Metallic Materials" held at MPIE with 70 participants, 02 Feb 2013

T. Hickel organized the Hydramicros meeting in Düsseldorf, 05 - 06 Feb 2013

T. Hickel co-organized an international workshop on "Unary Systems" at Ringberg Castle, 24 - 29 Mar 2013

J. Neugebauer co-organized a symposium on "Combinatorial Materials Science" at the spring meeting of the German Physical Society (DPG) in Regensburg, 11 - 15 Mar 2013

B. Grabowski and *J. Neugebauer* organized a symposium on "Computational Thermodynamics and Kinetics" at the TMS conference in San Antonio (USA), Mar 2013

M. Todorova, C. Freysoldt, and J. Neugebauer organized an international workshop on „Connecting electrochemical and water simulations: Status and future challenges" at Ringberg Castle, 21 - 24 Apr 2013

G. Dehm organized the "Mechanics meets Energy I" workshop between young scientists from the Ludwig-Maximilians-Universität, Munich and MPIE, Düsseldorf, 15 and 16 May 2013

L. Lymperakis organized the Alight EU project meeting in Düsseldorf, 05 Jun 2013

G. Dehm organized the GDRI CNRS Mecano "Mechanics of Nano-Objects" General Meeting in Düsseldorf, 18 and 19 Jul 2013

F. Roters organized the meeting of the Fachausschuss Computersimulation of the DGM entitled "Methoden der Gefügesimulation" held at Ruhr-Universität Bochum, 18 Aug 2013

J. Neugebauer co-organized a symposium on "Materials Discovery and High-Throughput Methods in Modelling and Experiment" at Euromat in Sevilla (Spain), 08 - 13 Sep 2013

G. Dehm was organizer for the topic "Mechanical Characterization" at EUROMAT 2013 in Sevilla, Spain, 8 - 13 Sep 2013

R. Spatschek co-organized an international summer school on phase field modeling in Peyresq (France) during 23 Sep – 04 Oct, 2013

M. Palm and F. Stein co-organized the international conference Intermetallics 2013 at the Educational Center Kloster Banz, Bad Staffelstein, 30 Sep - 04 Oct 2013

A. Erbe, C. Arckel and *C.D. Fernández-Solis* organised the training course "Optical spectroscopy at interfaces and in microfluidic channels" for fellows of the Marie Curie Initial Training Network "Somatai" at MPIE from 9 - 13 Dec 2013

2014

G. Dehm and *S. Brinckmann* organized the workshop "Mechanics meets Energy II" in Winterberg, Germany, 20 - 23 Jan 2014

Y. Li organized the first pearlite workshop held at MPIE, 10 - 11 Feb 2014

M. Palm organized and chaired the Intermetallics Technical Committee Meeting of the Deutsche Gesellschaft für Materialkunde (DGM) at MPIE, Düsseldorf, 26 Feb 2014

C. Kirchlechner organized the DGM-Arbeitskreis meeting "Rasterkraftmikroskopie und nano-mechanische Methoden", Düsseldorf, Germany, 27 - 28 Feb 2014

J. Neugebauer co-organized a symposium on "Thermodynamics and Kinetics on the Nanoscale" at the spring meeting of the German Physical Society (DPG) in Dresden, 30 Mar - 04 Apr 2014

B. Kohlhaas organized the MPIE Alumni Meeting "Applied fundamental research for nearly 100 years" on the occasion of the 60th Birthday of Prof. Martin Stratmann which took place at MPIE on 28 May 2014

F. Roters organized the 4th International Symposium on Computational Mechanics of Polycrystals, CMCn 2014 held at MPIE with 40 participants, 14 – 15 Jun 2014

M. Valtiner and *S. Brinkmann* organised the workshop "Bridging Scales in Tribology and Wear" at MPIE on 25 Jun 2014

G. Dehm and *C. Scheu* organized a meeting on "Merging Atomistic and Continuum Analysis of Nanometer Length-Scale Metal-Oxide Systems for Energy and Catalysis Applications (MACAN)" at MPIE Düsseldorf, 30 Jun - 2 Jul 2014

M. Todorova and J. Neugebauer co-organized an ICMR workshop on "Ab-initio description of charged systems and solid/liquid interfaces for semiconductors and electrochemisty" in Santa Barbara (USA), 07 - 11 Jul 7 2014

S. Zaefferer and *K. Angenendt* co-organized the meeting „Mikrostrukturcharakterisierung im Rasterelektronenmikroskop" at the BAM Berlin with 120 participants 08 - 09 Jul 2014

A. Erbe co-organized the summer school "Soft Matter at Aqueous Interfaces" in Berlin, Germany, 15 - 25 Aug 2014

T. Hickel co-organized a symposium (mini-colloquium) on "Structure and Dynamics – Metals" at the Condensed Matter in Paris CMD 25 – JMC 14 conference, Paris (France), 24 - 29 Aug 2014

G. Dehm co-organized the symposium "Structure and dynamics V: Mechanical properties at small scales" at the Condensed Matter conference CMD25 - JMC14 in Paris, France, 24 - 29 Aug 2014

M. Friák organized a symposium "Atomistic Origin of Ductility" at the Materials Science and Engineering (MSE) Congress 2014, Darmstadt (Germany), 23 -25 Sep 2014

C. Kirchlechner co-organized the Summer School „Theory and Practice of Modern Powder Diffraction", Ellwangen, Germany, 5 - 8 Oct 2014

J. Neugebauer co-organized a symposium on "Multiscale Simulations and Modeling for Integrated Materials Engineering" at the MMM conference in Berkeley (USA), 06 - 10 Oct 2014

T. Hickel and *J. Neugebauer* organized an ADIS workshop on "Ab initio Description of Iron and Steel: Multiple Impacts of Magnetism" at Ringberg Castle during 26 - 31 Oct 2014

M. Valtiner was member of the advisory board and chaired one symposium at the 2nd International Conference of Young Researchers on Advanced Materials (IUMRS-ICYRAM), in Haikou, Hainan, China from 24 - 29 Oct 2014

2015

M. Todorova organized the 2nd German-Austrian workshop on "Computational Materials Science on Complex Energy Landscapes" in Kirchdorf (Austria) from 19 - 23 Jan 2015

D. Ponge and Z. Tarzimoghadam organized the workshop on "Hydrogen Embrittlement and Sour Gas Corrosion in Oil and Gas Industry", held at MPIE with 80 participants, 27 - 28 Jan 2015

L. Lymperakis organized an Alight-Project Meeting in Düsseldorf, 16 - 17 Feb 2015

C. Kirchlechner co-organized the DGM-Arbeitskreis meeting "Rasterkraftmikroskopie und nanomechanische Methoden", Darmstadt, Germany 5 - 6 Mar 2015

T. Hickel co-organized a symposium on "Hydrogen in metals" at the spring meeting of the German Physical Society (DPG) in Berlin, 16 - 18 Mar 2015

G. Dehm, C. Scheu, and *S. Brinckmann* organized the "Mechanics meets Energy III" workshop in Burg Ebernburg, Germany, 23 - 26 Mar 2015

E. Gattermann and A. Erbe organised the workshop "Interface-controlled materials in energy conversion" of the IMPRS SurMat at the MPIE on 27 Apr 2015

C. Tasan organized the 3rd Int. Workshop on Physics Based Material Models and Experimental Observations, Cesme/Turkey. 02 - 04 Jun 2015

R. Hadian and *B. Grabowski* organized an international workshop on “Understanding Grain Boundary Migration“ in Reisensburg, 21 -24 Jun 2015

R. Spatschek organized a project meeting on press hardening in Düsseldorf, 01 Jul 2015

G. Dehm co-organized the symposium “Experimental Micromechanics and Nanomechanics” at the 9th European Solid Mechanics Conference ESMC 2015, Madrid, Spain, 6 - 10 Jul 2015

J. Neugebauer organized the 5th Sino-German Symposium on “Thermodynamics and Kinetics of Nano- and Mesoscale Materials and Their Applications“ in Changchun (China), 26 - 31 Jul 2015

G. Dehm co-organized the symposium “Metals, Alloys and Intermetallics” at the Microscopy Conference 2015, Göttingen, Germany, 6 - 11 Sep 2015

C. Tasan was coordinator of the Symposium “In-situ Micro- and Nano-Mechanical Characterization and Size Effects” at the EUROMAT 2015 in Warsaw/Poland, 20 - 24 Sep 2015

M. Palm and F. Stein co-organized the international conference Intermetallics 2015 at the Educational Center Kloster Banz, Bad Staffelstein, 28 Sep - 02 Oct.0 2015.0

Y. Li organized the second pearlite workshop held at MPIE, 20 - 21 Oct 2015

J. Neugebauer co-organized the ISIS Workshop in Moscow (Russia), 25 - 31 Oct 2015

J. Neugebauer co-organized the CECAM-Workshop Simulation of chemistry-driven growth phenomena for metastable materials in Rauischholzhausen, Germany, 08 -11 Nov 2015

M. Palm co-organized and chaired the symposium “Frontiers in Intermetallics” as part of the international Advances in Materials & Processing Technologies conference AMPT 2015, Madrid, Spain, 14 - 17 Dec 2015

Institute Colloquia and Invited Seminar Lectures

2013

M. Finnis, Imperial College London, UK: Grain Boundaries and Defects in Oxides (7 Jan 2013)

H. Boeckels, Clemson University, SC, USA: Effect of Oxygen on the Omega Stability in Metastable Beta Titanium Alloys (09 Jan. 2013)

K. Morgenstern, Uni Bochum: Properties of Nanosized Islands and Their Influence on Non-adiabatic Reactions (08 Jan. 2013, Colloquium)

V. Klinger, Fraunhofer-Institut für Solare Energiesysteme ISE, Gelsenkirchen: Multiple Solar Cells from III-V Semiconductors - Concept and Applications (14 Jan. 2013)

A. Tkatchenko, FHI Berlin: Many-Body van der Waals Interactions with Applications in Biology, Chemistry, and Physics (15 Jan. 2013)

R. Schäublin, Ecole Polytechnique Fédérale de Lausanne, Switzerland: Nanometric Defects in Metals in Transmission Electron Microscopy (17 Jan. 2013)

D. Terentyev, SCK-CEN, Nuclear Materials Institute, Mol, Belgium: Modelling Activities to Rationalize, Support and Design New Irradiation Experiments for Structural Steels (17 Jan. 2013)

S. Roy, Institut für Werkstoffwissenschaft und Werkstofftechnik, Chemnitz University of Technology: Role of Boron on the Evolution of Microstructure and Texture in Ti-6Al-4V-0.1B Alloy (21 Jan. 2013)

C. Kirchlechner, Montanuniversität Leoben, Austria: *In situ* Micromechanics: An Overview on Synchrotron based Experiments (21 Jan. 2013)

G. Grimvall, KTH Stockholm, Sweden: Lattice Instabilities in Metallic Alloys (24 Jan. 2013)

R. Raghavan, EMPA – Swiss Federal Laboratories for Materials Testing and Research, Dübendorf, Switzerland: Small Scale Mechanical Behavior of Amorphous Alloys, Wood and Multilayered Thin Films (28 Jan. 2013)

J. Wheeler, EMPA – Swiss Federal Laboratories for Materials Testing and Research, Dübendorf, Switzerland: *In situ* Nanomechanics at Elevated Temperature and Its Application to Crystalline Materials (28 Jan. 2013)

H. Biermann, TU Freiberg: TRIP-Matrix-Composite (30 Jan. 2013, Colloquium)

A.H. Heuer, Case Western Reserve University, Cleveland, OH, USA: Paraequilibrium Carburization of Austenitic Stainless Steels - Interstitial Hardening Taken to a New Level (18 Feb. 2013, Colloquium)

G. Richter, Max-Planck-Institut für Intelligente Systeme: Micro-/Nanostructure Formation by Physical Vapor Deposition (18 Feb. 2013)

B. Sanyal, Uppsala University, Sweden: Novel Magnetic Properties with Rare Earths in Thin Films & Clusters (22 Feb. 2013)

H. Sawada, Nippon Steel & Sumitomo Metal Corporation, Japan: First-principles Study of the Interface between Iron and Precipitates (25 Feb. 2013)

S. Ii, Structural Materials Unit, National Institute for Materials Science (NIMS), Tsukuba, Japan: Development of Nano Scale Quantitative Analyses by Transmission Electron Microscope and Its Application to Lattice Defects in Metals (12 Mar. 2013)

U. Guder, Çanakkale Onsekiz Mart University, Çanakkale, Turkey: Iron Metallurgy in Anatolia in the Middle Ages (15 Mar. 2013)

V. Heine, Cavendish Laboratory (TCM), U.K.: Theoretical Chemistry of Metallic Cohesion (19 Mar. 2013)

B. Braunschweig, Friedrich-Alexander-Universität Erlangen-Nürnberg: Study of Electrode/Electrolyte Interfaces by Sum Frequency Generation Spectroscopy (20 Mar. 2013)

A.E. Ismail, RWTH Aachen University: Improved Molecular Simulations of Interfaces (21 Mar. 2013)

P.E.A. Turchi, Lawrence Livermore National Laboratory: Thermodynamics of Alloys: The Road from *ab initio* to Phenomenology (21 Mar. 2013)

M.P. Moody, University of Oxford, UK: A Nexus between 3D Microscopy and Atomistic Simulation (26 Mar. 2013)

D. Holec, Montan-Universität Leoben, Austria: Texture Influence on Elastic Constants of Nitride Alloys (27 Mar. 2013)

E. Rabkin, Technion – Israel Institute of Technology, Haifa, Israel: From Thin Films to Nanoparticles: Microstructure, Kinetics, Mechanics (3 Apr. 2013)

C. Motz, Universität Saarbrücken: Influence of Defect Structure, Interfaces and Environment on the Micro-/ Nanomechanical Behavior of Metals (5 Apr. 2013)

M.T.M. Koper, Leiden Institute of Chemistry, Leiden University, The Netherlands: Electrocatalysis: From Single Crystals to Single Nanoparticles (09 Apr. 2013, Colloquium)

M. Mrovic, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg: Diffusion of Hydrogen in Strained Fe and Ni Lattices (10 Apr. 2013)

Z. Strelcova, Masaryk University, Brno, Czech Republic: The Theoretical Investigation of Chitin Nanofibrils Mechanical Properties (11 Apr. 2013)

T. Horiuchi, Hokkaido Institute of Technology, Sapporo, Japan: Effect of Alloying Elements on the Ordering Tendency in Alloy 690 based upon Thermodynamic Calculation (18 Apr. 2013)

T. Horiuchi, Hokkaido Institute of Technology, Sapporo, Japan: Experimental Study on Phase Equilibria in the Vicinity of X, W and H Phases in the Mg-Zn-Y Ternary System (18 Apr. 2013)

O. Hellman, Linköping University, Sweden: Temperature Dependent Effective Potential Method for Thermal Properties of Solids (23 Apr. 2013)

A. Heuer, Case Western Reserve University, Cleveland, OH, USA: On the Growth of Al_2O_3 Scales (26 Apr. 2013)

J.N. Israelachvili, UC Santa Barbara, CA, USA: Recent Work on Interesting Physico-Chemical Phenomena when Two Surfaces Slide Past Each Other (30 Apr. 2013, Colloquium)

C. Nishimura, National Institute for Materials Science, Tsukuba, Japan: Vanadium-based Alloy Design for Hydrogen Purification Membrane (13 May 2013)

Y. Fukai, Institute of Industrial Science, The University of Tokyo, Japan: Hydrogen-Induced Superabundant Vacancies – Coming Out of the Shade (14 May 2013, Colloquium)

C. Liebscher, University of California, Berkeley, CA, USA: Hierarchical Microstructure of Ferritic Alloys Strengthened By Two-phase $L2_1$-Ni_2TiAl / B2-NiAl Precipitates (17 May 2013)

S. Miura, Hokkaido University, Sapporo, Japan: Effects of the Alloying Elements on the Microstructure Control of Nb-Si Alloys (21 May 2013)

S.V. Divinski, University of Münster: Grain Boundary Diffusion: From Perfect Bicrystals to Severely Deformed Polycrystalline Materials (22 May 2013)

J. Deconinck, Vrije Universiteit Brussel, Belgium: Steps towards the Simulation of Atmospheric Corrosion (24 May 2013)

M. Kühbach, RWTH Aachen: Modeling Microstructure Evolution during Primary Static RX with Massively Parallelized Cellular Automata (3 June 2013)

U. Braun, Department of Law and Ethics of the Sciences, General Administration Max Planck Society, Munich: Good Scientific Practice (5 June 2013)

K.C. Jena, École Polytechnique Fédérale de Lausanne, Switzerland: Nonlinear Sum Frequency Vibrational Spectroscopy and its Relevance for Probing Interfacial Structure at Hidden Soft and Planar Interfaces (18 June 2013)

J. Behler, Ruhr-Universität Bochum: Interatomic Potentials for Molecules, Solids, and Surfaces Based on Artificial Neural Networks (19 June 2013)

M. Lazar, Darmstadt University of Technology: Non-singular Dislocation Fields in the Theory of Gradient Elasticity (21 June 2013)

R.C. Reed, University of Oxford, UK: On the Role of Numerical Modelling for Materials Technology for High Temperature Applications (25 June 2013)

L.-Q. Chen, Pennsylvania State University, State College, PA, USA: Kinetic Pathways of Phase Transformations and Microstructure Evolution in Two-phase Titanium Alloys (25 June 2013)

Z.-K. Liu, Pennsylvania State University, State College, PA, USA: High throughput CALPHAD modeling and the Materials Genome® (25 June 2013)

C.W. Sinclair, The University of British Columbia, Vancouver, Canada: Carbon Redistribution and Metastable Phases in Fe-C Alloys (26 June 2013)

C.W. Sinclair, The University of British Columbia, Vancouver, Canada: Microscale Plastic Strain Distribution in Slip Dominated Deformation of a ZEK 100 Mg-RE Alloy (27 June 2013)

P. Rinke, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin: Hybrid Organic/Inorganic Systems from First Principles (27 June 2013)

R. Hadian, Mc. Master University, Hamilton, Canada: Cementite Crystallography in Bainite (28 June 2013)

A. Wimmer, Erich Schmid Institute of Materials Science, Leoben, Austria: In-situ EBSD on Cu Micron-Lines (1 July 2013)

T.R. Bieler, Michigan State University, East Lansing, MI, USA: Characterization and Modeling of the Influence of Mesotexture on Heterogeneous Deformation in Ti and Ta (1 July 2013)

T. Tanaka, Nippon Steel & Sumitomo Metal Corporation, Chiba, Japan: Grain boundaries and interface characterization by AES and SIMS (1 July 2013)

S.H. Donaldson, University of California, Santa Barbara, CA, USA: Development of a General Interaction Potential for Hydrophobic and Hydrophilic Interactions (9 July 2013)

D. Trinkle, Univ. of Illinois at Urbana-Champaign, IL, USA: Deformation in Magnesium from First-Principles (10 July 2013, Colloquium)

G. Sha, The University of Sydney, Australia: Atom Probe Tomography for New Insights into Solute Nano-structures in Light Metals (29 July 2013)

U. Lienert, Deutsches Elektronen Synchrotron, Hamburg, Materials Characterization by High Energy Synchrotron Radiation (5 Aug. 2013)

X. Tao, Nanning University China: Physical Properties of Some Intermetallics from First-Principles Calculations (5 Aug. 2013)

M. Finnis, Imperial College London, UK: On the Growth of Alumina Scale (26 Aug. 2013)

C. Kübel, Karlsruhe Institute of Technology (KIT): New Approaches for Quantitative Electron Microscopic Characterization of Structural Changes in Nanocrystalline and Amorphous Metals during Mechanical Deformation (27 Aug. 2013)

E. McEniry, ICAMS Bochum: Toward Linear-Scaling Tight-Binding for Complex Metallic Alloys (28 Aug. 2013)

J. Takahashi, Nippon Steel & Sumitomo Metal Corporation, Chiba, Japan: Atom Probe Tomography Analysis of Severely Deformed Pearlitic Steels (5 Sep. 2013)

N. Park, Kyoto University, Japan: Dynamic Ferrite Transformation in Fe-6Ni-0.1C Alloy (11 Sep. 2013)

N. Park, Kyoto University, Japan: Strengthening in a Nano-Structured High-Entropy CrMnFeCoNi Alloy (12 Sep. 2013)

D. Weygand, Karlsruhe Institute of Technology (KIT), Karlsruhe: From Atomistic to Discrete Dislocation Dynamics Modelling of bcc Metals: Deformation of Tungsten (17 Sep. 2013)

F. Otto, University of Tennessee, Oak Ridge National Laboratory, Oak Ridge, TN, USA: The CoCrFeMnNi High-entropy Alloy: Phase Stability Aspects and Tensile Properties (20 Sep. 2013)

X. Banquy, Université de Montréal, Montréal, Canada: Bio-Inspired Lubrication: New Strategies and Future Prospects (20 Sep 2013)

S. Botti, Institut Lumière Matière (ILM) – CNRS, Université Claude Bernard Lyon 1, Villeurbanne, France: Designing and Understanding Novel Materials for Energy (23 Sep. 2013)

J. Van Humbeeck, MTM - KU Leuven, Belgium: Additive Manufacturing (AM) of Metallic Parts by Selective Laser Melting (SLM) (24 Sep. 2013, Colloquium)

F. Hausen, INM - Leibniz Institute for New Materials, Saarbrücken / University of Oxford, Oxford, UK: Atomic Friction in an Electrochemical Environment (24 Sep. 2013)

Y. Morimoto, Toyota Central R&D Labs., Inc, Nagakute, Aichi, Japan: Present Status of Fuel-Cell Powered Vehicles and Recent Topics on Electrocatalysis (24 Sep. 2013)

D. Barbier, Arcelormittal Maizières Research SA, Maizières les Metz, France: Interactions between Ferrite Recrystallization and Austenite Formation in High Strength Steels (4 Oct. 2013)

M. Takeyama, Tokyo Institute of Technology, Japan: Role of Grain-boundary TCP Laves Phase in Mechanical Properties of Novel Austenitic Heat Resistant Steels (7 Oct. 2013)

S. Kobayashi, National Institute for Materials Science, Tsukuba, Japan: The Formation of Fine Laves Phase Particles through Interphase Precipitation in Heat Resistant Ferritic Alloys (8 Oct. 2013)

V. Jayaram, Indian Institute of Science, Bangalore, India: Microscale Evaluation of Uniaxial and Fracture Behaviour of Bond Coats and the Role of Platinum (14 Oct. 2013, Colloquium)

S. Maisel, Technische Universität Hamburg-Harburg: Configuration Resolved High-Throughput Screening in Metal Alloys (28 Oct. 2013)

P. Suquet, LMA-CNRS, Marseille, France: A Computational Method Based on Fast Fourier Transforms for Heterogeneous Materials with Complex Microstructure (5 Nov. 2013, Colloquium)

G. Hautier, Université catholique de Louvain, Belgium: Accelerating Materials Discovery through High-Throughput Computing and the Materials Project (5 Nov. 2013)

P. Voyles, University of Wisconsin-Madison, WI, USA: Fluctuation Electron Microscopy Studies of Nanoscale Order in Metallic Glasses (13 Nov. 2013, Colloquium)

G. Laplanche, Ruhr-Universität Bochum: On the Stress Induced Formation of Martensite in NiTi Shape Memory Alloys during Nanoindentation (13 Nov. 2013)

C.-D. Nguyen, Ruhr-Universität Bochum: Interaction between Solid-Melt Interfaces and Gamma Surfaces (20 Nov. 2013)

P.A. Gruber, Karlsruhe Institute of Technology (KIT), Karlsruhe: Synchrotron-based *in situ* Mechanical Testing of Nanocrystalline Metals and Alloys (26 Nov. 2013)

L.P.H. Jeurgens, EMPA - Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland: Surprises at Interfaces in Nanomaterials (27 Nov. 2013)

P. Gurikov, Technische Universität Hamburg-Harburg: Mass Transfer in Disordered Media: A Cellular Automata Approach (28 Nov. 2013)

2014

C. Ayas, Cambridge University, Cambridge, UK: Climb Enabled Discrete Dislocation Plasticity (24 Jan. 2014)

M. Özaslan, Paul Scherrer Institut, Villigen, Switzerland: Pt Alloy Electrocatalysts for Oxygen Reduction Reaction (24 Jan. 2014)

U. Yalcin, Ruhr-Universität Bochum: Metallhandwerk in Anatolien: Anfänge und Entwicklung der Metallnutzung in Anatolien (27 Jan. 2014)

P. Krogstrup, Niels Bohr Institute, Copenhagen, Denmark: Nanowires – Growth, Characterization and Applications (28 Jan. 2014)

T. Detzel, Infineon Technologies AG, Villach, Austria: Innovative Semiconductor Solutions for Energy Efficiency, Mobility and Security – Products, Technologies and New Semiconductor Materials (30 Jan. 2014)

M. Nelhiebel, KAI - Kompetenzzentrum Automobil- und Industrieelektronik GmbH, Villach, Austria: REL4POWER - Research on Power Technology Reliability at Infineon Austria and KAI (30 Jan. 2014)

M. Sugiyama, Nippon Steel & Sumitomo Metals Corporation (NSSMC), Tokyo, Japan: Recent Activities for Characterization of Steel Microstructure in NSSMC (10 Feb. 2014)

A. Taniyama, Nippon Steel & Sumitomo Metals Corporation (NSSMC), Tokyo, Japan: 3D Analysis of Plastic Strain Propagation in Metallic Materials by 3D-EBSD (10 Feb. 2014)

D. Verreault, Ohio State University, Columbus, OH, USA: Probing Water Organization and Ion Distributions at Aqueous Interfaces by Vibrational Nonlinear Spectroscopy (10 Feb. 2014)

H. Clemens, University of Leoben, Austria: Development Status and Perspectives of Advanced Intermetallic Titanium Aluminides (13 Feb. 2014, Colloquium)

A. Wieck, Ruhr-Universitaet Bochum: Molecular Beam Epitaxy and Focussed Ion Beams (17 Feb. 2014)

H. Rösner, Westfälische Wilhelms-Universität Münster, A Novel Experimental Approach to Determine Density Changes in Shear Bands of Metallic Glasses by Correlative Analytical TEM (19 Feb. 2014)

D.A. Molodov, RWTH Aachen: Recent Investigations into Dynamics of Individual Grain Boundaries in Metals (27 Feb. 2014)

A. Duff, Imperial College London, UK: Finite Temperature Modelling of ZrC, HfC, ZrB2 and HfB2 (4 Mar. 2014)

T. Pardoen, Université catholique de Louvain, Louvain-la-Neuve, Belgium: Size and Rate Dependent Ductility of Thin Metallic Films (5 Mar. 2014)

T. Heinzel, Heinrich-Heine-Universität Düsseldorf: Electronic Transport in Inhomogeneous Magnetic Fields (14 Mar. 2014)

M. Sterrer, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin: Surface Science Models of Heterogeneous Catalysts – Probing Metal-Support Interaction with XPS and Auger Parameter Analysis (24 Mar. 2014)

Y. Ikeda, Kyoto University, Japan: Phonon Softening in Paramagnetic bcc Iron and Relationship with Phase Transition (24 Mar. 2014)

E. Spiecker, Friedrich-Alexander-Universität Erlangen-Nürnberg: From Graphite to Graphene: How Size Affects the Structure of Dislocations (2 Apr. 2014)

B. Sarac, Helmholtz-Zentrum Geesthacht and Hamburg University of Technology (TUHH): Toughening Mechanism of Advanced Microstructures: Experimental and Computational Approach (4 Apr. 2014)

K. Ogle, Ecole Nationale Supérieure Chimie Paris, Paris, France: Atomic Emission Spectroelectrochemistry: A New Look at the Corrosion, Dissolution and Passivation of Complex Materials (8 Apr. 2014, Colloquium)

T.J.J. Müller, Heinrich-Heine-Universität Düsseldorf: Functional Dyes on the Basis of Phenothiazines - Luminescent Electrophores in Solution, on Surfaces, and in Hybridmaterials (6 May 2014)

S.R. Kalidindi, Georgia Institute of Technology, Atlanta, Georgia: Microstructure Informatics for Mining Structure-Property-Processing Linkages from Large Datasets (7 May 2014, Colloquium)

S. Takagi, JFE Steel Corporation, Steel Research Laboratory, Kawasaki, Japan: Hydrogen Embrittlement Fracture Behavior of Ultra High Strength Steels (8 May 2014)

J. Möller, University Erlangen-Nürnberg: Atomistic Simulations of Fracture in bcc-Iron: Influence of the Interatomic Potential and Crack Front Curvature (13 May 2014)

A. Bachmaier, Universität des Saarlandes, Saarbrücken: The Formation of Supersaturated Solid Solutions in Immiscible Alloys Processed by Severe Plastic Deformation (15 May 2014)

T. Shao, State Key Laboratory of Tribology (SKLT) , Tsinghua University, Beijing, China: Advances in Thin Solid Coatings (6 June 2014)

J.T.M. De Hosson, University of Groningen, The Netherlands: Metallic Muscles at Work (11 June 2014, Colloquium)

R. Adharapurapu, GE India Technology Center, Bangalore, India: Effective Hf-Pd Co-doped β-NiAl(Cr) Coatings for Single Crystal Superalloys: A Combinatorial Investigation (16 June 2014)

H. Tueysuez, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr: Electrochemical Water Oxidation over Non-Noble Ordered Mesoporous Metal Oxides (18 June 2014)

P. Kejzar, Technical University of Liberec, Czech Republic: Structure and High Temperature Mechanical Properties of Ternary Fe-Al-Zr-type Intermetallic Alloys (24 June 2014)

W. Windl, Ohio State University, Columbus, Ohio, USA: Surface Modification and Oxidation of Graphene and Novel 2D Materials (27 June 2014)

N.P. Padture, Brown University, Providence, RI, USA: Thermal Barrier Coatings for High-Efficiency Gas-Turbine Engines in Aircraft and Power Plants (30 June 2014)

K. Limmer, Missouri University of Science and Technology, USA: Capabilities of DFT for Steel Alloy Design (1 July 2014)

B. Roldan, Ruhr-University Bochum: Nanocatalysts at Work (9 July 2014)

M. De Graef, Carnegie Mellon University, Pittsburgh, USA: Forward Modeling and a New Dictionary Approach to EBSD Pattern Indexing (16 July 2014)

A. Stark, Max Planck Institute of Colloids and Interfaces, Potsdam-Golm: More than 'just Carbon' - With N-Doping to Sustainable Metallic Coatings & Composites (24 July 2014)

K. Artyushkova, University of New Mexico, Albuquerque, NM, USA: Design Levers for Performance and Durability of Catalyst Layers (28 July 2014)

M. Bamberger, Technion – Israel Institute of Technology, Haifa, Israel: Cost-Effective High-Performance Materials & Processes (6 Aug. 2014)

P. Zabierowski, Warsaw University of Technology, Poland: Electrical Characterization of CIGS-based Solar Cells (7 Aug. 2014)

B. Kaplan, KTH Royal Institute of Technology, Stockholm, Sweden: Thermodynamics of Cr-Containing Cemented Carbides (18 Aug. 2014)

A. Blomqvist, Sandvik Coromant, Stockholm, Sweden: From Atomistic Modelling to Cutting Tool Performance (19 Aug. 2014)

S.H. Oh, POSTECH, Pohang, Korea: Role of Nano-Scale Twins in Deformation Processes of Metal Nanowires and Sea Shells (20 Aug. 2014)

L. Dézerald, CEA, DEN, Service de Recherches de Métallurgie Physique, Gif-sur-Yvette, France: *Ab initio* Modelling of Screw Dislocations in bcc Transition Metals (25 Aug. 2014)

N. Gurao, IIT Kanpur, India: Study of Heterogeneity of Plastic Deformation using Electron Back Scatter Diffraction and Synchrotron Micro-Diffraction (1 Sep. 2014)

J.B. Vogt, Lille University of Science and Technology, France: Fatigue of Alloys and of Metallic Alloys (4 Sep. 2014)

C. Reina, University of Pennsylvania, PA, USA: Atomistic Phase Field Model of Rapid Crystallization of Germanium from Amorphous Thin Films (5 Sep. 2014)

E.S. Park, Seoul National University, Seoul, Republic of Korea: Development of Bulk Metallic Glass Composites with "Super-elastic" Secondary Phase (11 Sep. 2014)

Z.-K. Liu, Pennsylvania State University, State College, PA, USA: Prediction of Diffusion Coefficients in Liquid and Solids (12 Sep. 2014)

W.-J. Li, Industrial Technology Research Institute, Hsinchu, Taiwan: Effects of Extrinsic Cupric on Pitting Corrosion of Aluminum Radiator (15 Sep. 2014)

G. Csanyi, University of Cambridge, UK: Phase Diagrams 'ex nihilo' (16 Sep. 2014)

S. Zhang, University of Cambridge, UK: Band Structures and Polarisations of Nonpolar GaN Light Emitting Diodes (18 Sep. 2014)

A. Ceguerra, Australian Centre for Microscopy & Microanalysis, The University of Sydney, Australia: Computational Atom Probe Microscopy – Chemical Microanalysis at the Atomic Scale (24 Sep. 2014)

D. Zander, RWTH Aachen: Influence of Alloying Elements and Microstructure on Corrosion of Magnesium Alloys (30 Sep. 2014)

M. Alam, TU Bergakademie Freiberg: Computational Study of Materials via Multiscale Modeling (2 Oct. 2014)

D.C. Lagoudas, Dept. of Aerospace Engineering, Texas A&M University, USA: Driving Force for Crack Growth and Toughness Enhancement in Shape Memory Alloy Actuators (10 Oct. 2014)

P. Albers, Kompetenzzentrum Elektronenmikroskopie/Oberflächenanalytik, AQura GmbH, Hanau: Hydrogen on and in Materials: Observations in Catalysis and Production Technology (27 Oct. 2014)

C. Greiner, Karlsruhe Institute of Technology (KIT), Karlsruhe: Materials Tribology: Grain Size Evolution of High-Purity Copper under Reciprocating Tribological Loading (28 Oct. 2014)

L. Kranz, EMPA - Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland: Cadmium Telluride Solar Cells in Substrate Configuration (31 Oct. 2014)

G. Schmitz, Institut für Materialwissenschaft, Universität Stuttgart: Understanding Atom Probe Tomography – A Theoretical Challenge (4 Nov. 2014, Colloquium)

D. Trinkle, University of Illinois at Urbana-Champaign, IL, USA: Forming Nanoprecipitates at Dislocations: Hydrides in Pd and Silicides in Ni (5 Nov. 2014)

R. Hennig, University of Florida, Gainesville, FL, USA: VASPsol: An Implicit Solvation Model for Density-Functional Calculations (6 Nov. 2014)

S. Korte-Kerzel, RWTH Aachen: Plasticity in Anisotropic and Brittle Materials - Testing at the Microscale and at High Temperatures (10 Nov. 2014)

M. Wu, Paul-Drude-Institut für Festkörperelektronik, Berlin, and Tampere University of Technology, Tampere, Finland: Alternative to Stranski-Krastanov Quantum Dots? Formation and Phase Transformation of Bi-Containing Quantum Dot-Like Clusters in Annealed GaAsBi (13 Nov. 2014)

M. Mikami, MCHC R&D Synergy Center, Inc., Yokohama, Japan: Theoretical Approach for White–LED (Oxy)Nitride Phosphors: State of the Art (13 Nov. 2014)

A. Davydok, IM2NP - UMR CNRS 7334 & Universities of Aix-Marseille and Toulon, France: X-Ray Diffraction Investigation of Mechanical Properties of Nanostructures (21 Nov. 2014)

M. Getzlaff, Heinrich Heine Universität Düsseldorf: Influence of Hydrogen to Nanoscaled Systems (25 Nov. 2014)

K. Doda, Northwestern University, Evanston, IL, USA: Tribology in Multi-Scale Metal Forming (28 Nov. 2014)

B. Alling, Linköping University, Linköping, Sweden: Modeling Magnetic Materials at High Temperature from First-Principles: Disordered Magnetism, Vibrations, Phase Stability, and Magnetic Exchange Interactions (10 Dec. 2014)

2015

M. Rabe, Universiteit Leiden, The Netherlands: New Pictures of an Old Motif: A Physical Chemists View on Coiled-Coil (9 Jan. 2015)

E. George, Ruhr-Universität Bochum: Phase Stability and Mechanical Properties of High- and Medium-Entropy Alloys (14 Jan. 2015, Colloquium)

B. Ziebarth, Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg: Atomistic Studies on the Interaction of Impurity Atoms with Extended Defects in Silicon (26 Jan. 2015)

S.I. Rao, EPFL, Lausanne, Switzerland: Large Scale 3-D Dislocation Dynamics and Atomistic Simulations of Flow and Strain-Hardening Behavior of Metallic Micropillars (5 Feb. 2015)

T. Mohri, Institute for Materials Research, Tohoku University, Sendai, Japan: Towards First-principles Continuous Displacement Cluster Variation Method within Computational Materials Science Projects in Japan (9 Feb. 2015, Colloquium)

S.W. D´Souza, Max Planck Institute for Chemical Physics of Solids, Dresden: Magnetic Properties and Electronic Structure of Mn-Ni-Ga Magnetic Shape Memory Alloys (9 Feb. 2015)

H. Cohen, Weizmann Institute of Science, Rehovot, Israel: Band Alignment & Charge Transport Mechanisms in CREM of ETA Solar Cells (10 Feb. 2015, Colloquium)

R. Hoffmann-Vogel, Karlsruhe Institute of Technology (KIT), Karlsruhe: High-Resolution Kelvin Probe Force Microscopy (12 Feb. 2015)

M. Garbrecht, Linköping University, Linköping, Sweden: Aberration-Corrected HR(S)TEM as an Ultra-Precise Tool in Materials Science (13 Feb. 2015)

W. Solano-Alvarez, University of Cambridge, Cambridge, UK: Microstructural Degradation of Bearing Steels under Rolling Contact Fatigue (17 Feb. 2015)

B.A. Szost, European Space Agency, Noordwijk, The Netherlands: Hydrogen Trapping in Bearing Steels: Mechanisms and Alloy Design (18 Feb. 2015)

M. Poková, Charles University, Prague, Czech Republic: Electron Microscopy Study of Aluminium Alloys Enhanced by Zr (23 Feb. 2015)

F. von Wrochem, Materials Science Laboratory, Sony Deutschland, Stuttgart: Insights into Work at the Research Facility of Sony in Germany (2 Mar. 2015)

G. Requena, German Aerospace Canter (DLR), Cologne: Research on Metallic Structures and Hybrid Materials Systems at the DLR (10 Mar. 2015)

R. Shiju, University of Amsterdam, The Netherlands: Catalysis in Action: A Few Short Stories (17 Mar. 2015)

J. Janßen, Technische Universität Kaiserslautern: An Atomistic Study of C in Alpha-Fe Grain Boundaries (27 Mar. 2015)

R. Hielscher, Technische Universität Chemnitz: MTEX - A Texture Calculation Toolbox (14 Apr. 2015)

K.F. Domke, Max Planck Institute for Polymer Research, Mainz: A Molecular View on Sensitized Solar Cells (14 Apr. 2015)

U. Pietsch, University of Siegen: Structure to Property Relations of Single MBE Grown GaAs and InAs Nanowires onto Silicon (111) by X-Ray Nanodiffraction (24 Apr. 2015)

C. Teichert, Montanuniversität Leoben, Leoben, Austria: Advanced AFM based Electrical Characterization on the Nanometer Scale (27 Apr. 2015)

J. Popovic, Max Planck Institute for Solid State Research, Stuttgart: Individual Contribution of the Ionic Species to the Ionic Conduction: From Lithium Containing Liquid to Liquid-Solid Composite Electrolytes (28 Apr. 2015)

D. Anselmetti, Bielefeld University, Bielefeld: Single Molecule Interaction Analysis: From Nanopores and Catch Bonds (30 Apr. 2015)

R. Reed, University of Oxford: Superplasticity in Ti-6Al-4V: Characterisation, Modelling and Applications (5 May 2015)

Y. Amouyal, Technion - Israel Institute of Technology, Haifa, Israel: Thermoelectric Materials Design via Microstructure and Composition Manipulations: Experimental and Computational Approaches (12 May. 2015, Colloquium)

T. Frolov, University of California, Berkeley, USA: Many Faces of Interfaces (13 May 2015, Colloquium)

P. Haynes, Imperial College London, UK: Linear-Scaling DFT and TDDFT with Optimised Local Orbitals and Plane-Waves (19 May 2015)

M. Militzer, The University of British Columbia, Vancouver, BC, Canada: Next Generation Phase Transformation Models for Advanced Low-carbon Steels (20 May 2015)

W. Wolf, Materials Design®, Paris, France: MedeA Software Package Applications (21 May 2015)

R. Griessen, VU University, Amsterdam, and Amsterdam University College, The Netherlands: Hydrogenography: Shedding Light on Switchable Metal-Hydride Mirrors (1 June 2015)

G. Wilde, Universität Münster: Shear Bands in Metallic Glasses: Atomic Mobility, Relaxation and Excess Volume (8 June 2015)

G. Langer, University of Cambridge, UK: Coccolithophores – With Special Emphasis on Calcification, Coccoliths, and Coccospheres (18 June 2015)

R. Hoffmann, Ludwig-Maximilians-Universität München: Coccolithophores – A View Inside on Coccolith Architecture and Crystallographic Orientation (18 June 2015)

J.C. Yang, University of Pittsburgh, PA, USA: Structural Dynamics of Surface Reactions: Oxidation and Heterogeneous Catalysis (19 June 2015)

D. Stroz, University of Silesia, Katowice, Poland: Progress in Understanding of Phase Transformations in NiTi Shape Memory Alloys (23 June 2015, Colloquium)

V.I. Levitas, Iowa State University, Ames, IA, USA: Interaction between Phase Transformations and Dislocations at the Nanoscale: Phase Field Approach (23 June 2015)

F.H. Akbary, TU Delft, The Netherlands: Assessment of Mechanical Properties in Quenching and Partitioning Steels (23 June 2015)

G. Gerstein, Leibniz Universität Hannover: The Electroplastic Effect in Metallic Materials - Former Investigations and Current Results (29 June 2015)

S. Wohletz, Technische Universität Darmstadt: Bond Formation by Cold Extension Welding (1 July 2015)

B. Sakar, Galgotias University, India: Finite-Temperature Lattice Dynamics of Binary Chalcogenides within the Quasi-Harmonic Approximation (16 July 2015)

C.G. Van de Walle, University of California, Santa Barbara, CA, USA: Oxides for Energy and Electronics (23 July 2015)

M. Finnis, Imperial College, London, UK: Thermodynamics of Interfaces (6 Aug. 2015)

S. Meka, Max-Planck-Institute for Intelligent Systems (formerly Max-Planck-Institute for Metals Research), Stuttgart: Nitriding Induced Microstructural Transformations in Iron-Based Alloys (12 Aug. 2015)

R. Nazarov, Lawrence Livermore National Lab, Livermore, CA, USA: *Ab initio* Calculations in Petaflop Era: Properties of Molecules, Metals and Insulators Computed with Chemical Accuracy using Quantum Monte Carlo (3 Sep. 2015)

B.P. Gorman, Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO USA: Adventures at the Atomic Scale: Diffusion and Defect Chemistry using Correlative STEM and Atom Probe Tomography (4 Sep. 2015)

P. Felfer, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nuremberg: New Insights into Interfaces of Metals, Oxides and Nanoparticles via APT (21 Sep. 2015)

J. Eckert, IKM Dresden: Tailoring Metastable Metallic Materials for Engineering Applications (14 Oct. 2015, Colloquium)

S.J.J. Sandoval, Centro de Investigación y de Estudios Avanzados del IPN, Unidad Querétaro, Mexico: Properties of CuCdTeO Films: From Solid Solutions to Composites (9 Nov. 2015)

C. Leinenbach, Laboratory for Joining Technologies and Corrosion, EMPA - Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland: Design and Characterization of Novel TiAl Alloys and Metal-Diamond Composites for Beam-based Additive Manufacturing (10 Nov. 2015)

K. Loza, Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CeNIDE), Essen: Nanostructure of Wet-Chemically Prepared, Polymer-Stabilized Silver–Gold Nanoalloys (6 nm) over the Entire Composition Range (10 Nov. 2015)

E. Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nuremberg: Atomistic Studies on Dislocation – Interface Interactions: from Planar Coherent Twin Boundaries to Curved Interphase Boundaries (7. Dec. 2015, Colloquium)

M. Sebastiani, Roma TRE University, Rome, Italy: Measurement of Fracture Toughness by Nanoindentation Methods: Recent Advances and Future Challenges (14. Dec. 2015)

Lectures and Teaching at University

2013

G. Dehm, Universität Salzburg, Austria, Materialwissenschaften 1, WS 2012/13

G. Dehm, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2013

G. Dehm, Ruhr-Universität Bochum: Advanced Transmission Electron Microscopy, WS 2013/2014

A. Erbe, Ruhr-Universität-Bochum: Spectroscopy of Surfaces and Interfaces, WS 2012/2013

A. Erbe, Ruhr-Universität-Bochum: Spectroscopy of Surfaces and Interfaces, WS 2013/2014

A. Erbe, M. Valtiner, M. Muhler, K.J.J. Mayrhofer, & M. Rohwerder, Ruhr-Universität-Bochum: Physical chemistry of surfaces and interfaces, Oct 2013

C. Freysoldt, A. Schindlmayr, Universität Paderborn: Computerphysik, WS 2013/14

T. Hickel, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2013/2014

C. Kirchlechner, University of Leoben: Metallkundliche Arbeitsverfahren, WS 2013/2014

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part I, WS 2012/2013

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2013

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part I, WS 2013/2014

J. Neugebauer, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2013

D. Raabe, RWTH Aachen: Micromechanics of Materials, SS 2013

D. Raabe, SurMat IMPRS Teaching, Max-Planck-School: Dislocation and Interfaces – Materials Mechanics, Mar 2013

M. Rohwerder, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2013/2014

M. Rohwerder, Ruhr-Universität Bochum: Surface Analysis and Characterization, WS 2013/2014

F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2012/2013

F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2013/2014

R. Spatschek, F. Varnik, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2013/2014

S. Zaefferer, T. Hickel, U. Prahl, RWTH Aachen: Microstructures, Microscopy & Modelling, SS 2013

S. Zaefferer, University of British Columbia, Vancouver, Canada: Textures, Microstructures and Microscopy, Summer course 2013

2014

G. Dehm, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2014

G. Dehm, Ruhr-Universität Bochum: Advanced Transmission Electron Microscopy, WS 2014/2015

A. Erbe, Ruhr-Universität-Bochum: Spectroscopy of Surfaces and Interfaces, WS 2014/2015

C. Freysoldt, Universität Paderborn: Quantenchemie, SS 2014

T. Hickel, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2014/2015

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2014

K.J.J.Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part I, WS 2014/2015

J. Neugebauer, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2014

D. Raabe, RWTH Aachen: Micromechanics of Materials, SS 2014

M. Rohwerder, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2014/2015

F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2014/2015

F. Roters, RWTH Aachen: ICME for Steels, WS 2014/2015

C. Scheu, RWTH Aachen: Electron Microscopy and Analytical Techniques, WS 2014/2015

R. Spatschek, F. Varnik, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2014/2015

M. Valtiner, Ruhr-Universität Bochum: Non-linear optics, SS 2014

S. Zaefferer, T. Hickel, U. Prahl, RWTH Aachen: Microstructures, Microscopy & Modelling, SS 2014

S. Zaefferer, Universität Wien, Austria: Textures, Microstructures and Microscopy, Autumn course 2014

2015

G. Dehm, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2015

G. Dehm, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2015/2016

T. Hickel, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2015/2016

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2015

K.J.J. Mayrhofer, M. Muhler, M. Valtiner, S. Wippermann, & M. Rohwerder, Ruhr-Universität-Bochum: Physical chemistry of surfaces and interfaces, Sept. 2015

J. Neugebauer, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2015

D. Raabe, SurMat IMPRS Teaching, Max-Planck-School: Dislocation and Interfaces – Materials Mechanics, March 2015

D. Raabe, RWTH Aachen: Micromechanics of Materials, SS 2015

M. Rohwerder, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2015/2016

M. Rohwerder, Ruhr-Universität Bochum: Surface Analysis and Characterization, WS 2015/2016

C. Scheu, RWTH Aachen: Advanced Characterization, SS 2015

R. Spatschek, F. Varnik, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2015/2016

S. Zaefferer, T. Hickel, U. Prahl, RWTH Aachen: Microstructures, Microscopy & Modelling, SS 2015

Invited Talks at Conferences and Colloquia

2012 (not included in Scientific Report 2011/2012)

Enax, J.; Prymak, O.; Fabritius, H.-O.; Raabe, D.; Epple, M.: *Shark teeth: Relating hierarchical structure, composition, and the resulting mechanical properties for bio-inspiration*. (Workshop: Biocompatible Coatings and their applications, University Duisburg-Essen and Evonik. Essen, Germany. 2012-09-13 to 2012-09-14).

Epple, M.; Enax, J.; Prymak, O.; Fabritius, H.-O.; Raabe, D.: *Shark teeth: Relating hierarchical structure, composition, and the resulting mechanical properties for bio-inspiration*. (Ringberg Symposium 2012: Generation of Inorganic Functional Materials - Implementation of Biomineralization Principles, Schloss Ringberg. Rottach-Egern, Germany. 2012-09-30 to 2012-10-03).

Grabowski, B.: *Quantitative Limits of DFT Phase Transitions: Importance of Anharmonicity, Point Defects and Exchange-Correlation Functionals*. (Workshop on "Simulation of Complex Microstructure Pathways for Alloy Design." McMaster University, Hamilton, Canada. 2012-11-29 to 2012-11-30).

Grabowski, B.; Tasan, C.: *Design of Adaptive Structural Materials: A coupled theoretical-experimental approach*. (10th Materials Day. Bochum, Germany. 2012-11-09).

Gutiérrez-Urrutia, I.: *Electron channelling contrast imaging under controlled diffraction conditions: A powerful technique for quantitative microstructural characterization of deformed materials*. (International Symposium on Plastic Deformation and Texture Analysis. Alcoy, Spain. 2012-09-24 to 2012-09-25).

Mayrhofer, K. J. J.: *Investigations of fuel cell electrocatalyst degradation - A fundamental perspective*. (Seminar lecture at Norwegian University of Science and Technology. Trondheim, Norway. 2012-11-01).

Mayrhofer, K. J. J.: *Scanning Flow Cell System for Fully Automated Screening of Electrocatalyst Materials*. (Seminar lecture at Danish University of Technology. Copenhagen, Denmark. 2012-10-11).

Neugebauer, J.: *Ab initio based free energy sampling*. (Workshop. Lake Arrowhead, CA, USA. 2012-12-10 to 2012-12-14).

Neugebauer, J.: *Introduction to Density Functional Theory from a Materials Science Perspective*. (Workshop. Lake Arrowhead, CA, USA. 2012-10-12 to 2012-10-14).

Neugebauer, J.: *Introduction to Density Functional Theory from a Materials Science Perspective*. (IPAM Workshop. Los Angeles, CA, USA. 2012-09-19).

Nikolov, S.; Fabritius, H.-O.; Friák, M.; Raabe, D.: *The Multiscale Modeling of Biomaterials as a Tool for Understanding the Design Principles in Nature*. (IVth National Crystallographic Symposium. Sofia, Bulgaria. 2012-11-01 to 2012-11-03).

Plancher, E.; Tasan, C. C.; Sandlöbes, S.; Raabe, D.: *Multi-scale characterization of the giant fault mechanism in Ti–Nb based gum cast alloys*. (12th Materials Science & Technology (MS&T) Conference. Pittsburgh, PA, USA. 2012-10-07 to 2012-10-11).

Ram, F.; Zaefferer, S.; Khorashadizadeh, A.; Jäpel, T.; Davut, K.: *Electron Diffraction in Scanning Electron Microscope and its applications*. (Institut für Werkstofftechnik, Helmut Schmidt Universität. Hamburg, Germany. 2012-11).

Rohwerder, M.: *Corrosion - Aqueous*. (Gordon Research Seminar: Corrosion - Aqueous, Colby-Sawyer College. New London, NH, USA. 2012-07-08 to 2012-07-13).

Springer, H.; Raabe, D.: *Rapid Alloy Prototyping - Effizientes Legierungsdesign durch kombinatorische Metallurgie und Prozesstechnik*. (Institutsseminar at IEhK - RWTH Aachen, Germany. 2012-12-13).

Springer, H.; Raabe, D.: *Rapid Alloy Prototyping - Effizientes Legierungsdesign durch kombinatorische Metallurgie und Prozesstechnik*. (VDEh Grundlagenausschuss Metallurgie. Düsseldorf, Germany. 2012-06-22).

Tasan, C. C.: *Multi-scale (in-situ) investigation of Adaptive Structural Materials*. (École Seminar, Nationale Supérieure des Mines de St-Étienne, France. 2012-09-20).

2013

Auinger, M.: *Phase Diagrams with FACTSage - Speaking different Languages for Thermochemical Properties.* (GTT-Workshop on Thermodynamic Simulations in Industry. Herzogenrath, Aachen, Germany. 2013-07-05).

Boehlert, C.; Chen, Z.; Gutiérrez-Urrutia, I.; Pérez-Prado, M. T.; Llorca, J.; Bohlen, J.; Yi, S.; Letzig, D.: *In-situ analysis of deformation and recrystallization mechanisms in magnesium alloys.* (International Symposium on Plasticity 2013. Nassau, Bahamas. 2013-01-03 to 2013-01-08).

Brinckmann, S.: *Combining Atomistic and Dislocation Dynamics into a Concurrent Multiscale Model.* (Seminar zur Physik der kondensierten Materie, Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany. 2013-07-09 to 2013-07-09).

Brinckmann, S.: *Deformation localization and strain hardening during micro shear experiments on gold in the SEM.* (Nanomechanical Testing in Materials Research and Development IV. Olhão (Algarve), Portugal. 2013-10-06 to 2013-10-11).

Brinckmann, S.: *Joining 3D Dislocation Dynamics and 3D Molecular Dynamics into a Concurrent Multiscale Model.* (SES 50th Annual Technical Meeting and ASME-AMD Annual Summer Meeting. Providence, RI, USA. 2013-07-28 to 2013-07-31).

Brinckmann, S.: *Discrete Disclination Dynamics in comparison to Discrete Dislocation Dynamics.* (SES 50th Annual Technical Meeting and ASME-AMD Annual Summer Meeting. Providence, RI, USA. 2013-07-28 to 2013-07-31).

Brinckmann, S.: *Discrete Disclination Dynamics & Discrete Dislocation Dynamics.* (4th International Conference on Ferromagnetic Shape Memory Alloys. Boise, ID, USA. 2013-06-03 to 2013-06-07).

Brinckmann, S.: *Studying very short cracks with a 3D multiscale model.* (DPG-Frühjahrstagung der Sektion Kondensierte Materie (SKM). Regensburg, Germany. 2013-03-10 to 2013-03-15).

Choi, P.-P.: *Characterization of internal interfaces in Cu(In,Ga)Se_2 thin-film solar cells using correlative microscopy.* (IEEE - Photovoltaic Specialist Conference. Denver, CO, USA. 2013-06-08 to 2013-06-13).

Choi, P.: *Characterization of κ-carbide precipitates in austenitic Fe–Mn–Al–C steels using atom probe tomography.* (Thermec 2013. Las Vegas, NV, USA. 2013-12-02 to 2013-12-06).

Choi, P.: *Atom Probe study of $Cu_2ZnSnSe_4$ thin-films prepared by co-evaporation and post-deposition annealing.* (Euromat 2013. Sevilla, Spain. 2013-09-08 to 2013-09-13).

Choi, P.: *Atomic-scale insights into thin-film solar cells by Atom Probe Tomography.* (Korean German Forum on Nanotechnology. Düsseldorf, Germany. 2013-08-28).

Choi, P.: *Overview of atom probe tomography research at MPIE.* (Seminar at the Ruhr University of Bochum, Germany. 2013-01-31).

Cojocaru-Mirédin, O.; Stoffers, A.; Würz, R.; Raabe, D.: *Role of internal interfaces in solar cells.* (International Workshop on Interface-dominated Materials. Bochum, Germany. 2013-10-21 to 2013-10-28).

Cojocaru-Mirédin, O.: *Atom Probe Tomography.* (2013 MRS Spring Meeting & Exhibit. San Francisco, CA, USA. 2013-04-01 to 2013-04-05).

Dehm, G.: *Atomic resolution interface study of VN and Cu films on MgO using Cs corrected TEM.* (Microscopy Conference MC 2013. Regensburg, Germany. 2013-08-25 to 2013-08-30).

Dehm, G.: *Struktur und Nano-/Mikromechanik von Materialien.* (Thüringer Werkstofftag. Ilmenau, Germany. 2013-03-21).

Dehm, G.: *Struktur und Nano-/Mikromechanik von Materialien.* (Vorstandssitzung des Stahlinstituts VDEh und der Wirtschaftsvereinigung Stahl. Düsseldorf, Germany. 2013-03-14).

Dehm, G.; Kirchlechner, C.; Imrich, P. J.; Smolka, M.; Wimmer, A. C.; Yang, B.; Zhang, Z.: *Plasticity and Fracture at Small Length Scales: From Single Crystals Towards Interfaces.* (Workshop on Mechanical Behaviour of Systems - 4. Coorg, Karnataka, India. 2013-02-24 to 2013-02-28).

Dehm, G.: *Mechanical Behavior of Materials with a Focus on Thin Films.* (MACAN-Infineon Idea Exchange Meeting 2013. Villach, Austria. 2013-01-15 to 2013-01-18).

Dehm, G.: *In situ Transmission Electron Microscopy.* (3rd School on Advanced TEM Quantitative Techniques. Saint-Aygulf, France. 2013-05-13 to 2013-05-24).

Dehm, G.: *On the atomic interface structure of a hard nitride coating on MgO.* (Nanostructured Multialyers 13. Madrid, Spain. 2013-09-30 to 2013-10-04).

Dehm, G.: *Probing deformation phenomena at small length scales.* (ECI on Nanomechanical Testing in Materials Research and Development IV. Olhão, Portugal. 2013-10-06 to 2013-10-11).

Dehm, G.: *Superhard, flexible, fatigue resistant: mechanical demands for thin films.* (Composites at Lake Louise 2013 (Composites 2013). Banff, Canada. 2013-11-03 to 2013-11-07).

Dehm, G.: *Struktur und Mikromechanik von Materialien.* (Materials Valley e.V. - Vortragsreihe Materialforum. Hanau, Germany. 2013-11-18).

Dehm, G.: *Structure and Micromechanics of Materials.* (Materialwissenschaftliches Kolloquium ICAMS und Institut für Werkstoffe, RUB. Bochum, Germany. 2013-11-28).

Dehm, G.: *From idealized bi-crystals towards applied polycrystals: Plastic deformation in small dimensions.* (2013 MRS Fall Meeting. Boston, MA, USA. 2013-12-01 to 2013-12-06).

Dutta, B.; Körmann, F.; Dey, P.; Hickel, T.; Neugebauer, J.: *Ab-initio based prediction of chemical trends for phase transitions in magnetic shape memory alloys.* (Weekly Seminar, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany. 2013-08-27).

Fabritius, H.-O.: *Structure-property relations in biological materials - Opportunities and challenges.* (Summer School of the SPP1420 at the University of Ulm, Germany. 2013-07-25 to 2013-07-26).

Freysoldt, C.; Pfanner, G.; Neugebauer, J.: *Defects in amorphous silicon from H insertion.* (Workshop “Spins as Functional Probes in Solar Energy Research”. Berlin, Germany. 2013-04-10 to 2013-04-12).

Friák, M.; Sandlöbes, S.; Pei, Z.; Zhu, L.-F.; Dick, A.; Wang, F.; von Pezold, J.; Zaefferer, S.; Yi, S.; Letzig, D.; Sheng, H. W.; Race, C. P.; Svendsen, B.; Raabe, D.; Neugebauer, J.: *Combined theoretical and experimental studies of ductile Mg alloys.* (International Symposium on Atomistic Modeling for Mechanics. Tokyo, Japan. 2013-07-22 to 2013-07-24).

Friák, M.; Sandlöbes, S.; Pei, Z.; Zhu, L.-F.; Dick, A.; von Pezold, J.; Zaefferer, S.; Hickel, T.; Yi, S.; Letzig, D.; Sheng, H. W.; Race, C. P.; Leyson, G.; Svendsen, B.; Raabe, D.; Neugebauer, J.: *Combined theoretical and experimental studies of ductile Mg alloys.* (Seminar lecture at the Technical University Bergakademie Freiberg, Germany. 2013-07-08).

Friák, M.; Petrov, M.; Nikolov, S.; Sachs, C.; Fabritius, H. O.; Hemzalová, P.; Ma, D.; Lymperakis, L.; Raabe, D.; Janus, A. M.; Hild, S.; Zigler, A.; Neugebauer, J.: *Arthropod cuticle: A biological multi-functional composite used as template for nano-to-macro-scale hierarchical modeling.* (7th International Conference on Materials Structure and Micromechanics of Fracture. Brno, Czech Republic. 2013-07-01 to 2013-07-03).

Friák, M.; Petrov, M.; Nikolov, S.; Sachs, C.; Fabritius, H. O.; Elstnerová, P.; Ma, D.; Lymperakis, L.; Raabe, D.; Hild, S.; Zigler, A.; Neugebauer, J.: *Arthropod cuticle: A biological multi-functional composite used as template for nano-to-macro-scale hierarchical modeling.* (Advanced Materials 2013. Zhenjiang, China. 2013-05-16 to 2013-05-19).

Grabowski, B.; Glensk, A.; Korbmacher, D.; Huang, L.; Körmann, F.; Hickel, T.; Neugebauer, J.: *First principles at finite temperatures: New approaches and massively parallel computations.* (CMSI International Symposium 2013: Extending the power of computational materials sciences with K-computer. Ito International Research Center, University of Tokyo, Japan. 2013-10-21 to 2013-10-22).

Grabowski, B.; Glensk, A.; Korbmacher, D.; Huang, L.; Körmann, F.; Hickel, T.; Neugebauer, J.: *First principles at finite temperatures: New approaches and massively parallel computations.* (IMR Seminar at Institute for Materials Research, Tohoku University. Sendai, Japan. 2013-10-22).

Gutiérrez-Urrutia, I.; Seol, J.-B.; Marceau, R. K. W.; Herbig, M.; Welsch, E.; Choi, P.; Raabe, D.: *High strength and ductile high-Mn low-density steels by ordered nanocarbides.* (Euromat 2013. Sevilla, Spain. 2013-09-08 to 2013-09-13).

Gutiérrez-Urrutia, I.; Raabe, D.: *Electron channelling contrast imaging under controlled diffraction conditions: A powerful technique to characterize deformation structures in the SEM.* (Euromat 2013. Sevilla, Spain. 2013-09-08 to 2013-09-13).

Herbig, M.; Goto, S.; Li, Y.; Choi, P.; Zaefferer, S.; Nematollahi, A.; Kirchheim, R.; Nikolov, S.; Friák, M.; Borchers, C.; Neugebauer, J.; Raabe, D.: *Nanostructures in 1 Billon Tons: Interface Engineering in Complex Steels and Biological Nanocomposites.* (Materialwissenschaftliches Kolloquium, Universität Hamburg-Harburg, Germany. 2013-07-03).

Hickel, T.; Dutta, B.; Körmann, F.: *What can we learn from theory about ferroic cooling?* (SPP1599 Convention. Schney, Germany. 2013-07-29 to 2013-08-01).

Hickel, T.: *Ab initio – Vom Atom zum Hochleistungswerkstoff.* (HdT – Tagung Hochleistungswerkstoffe. Essen, Germany. 2013-09-10).

Hickel, T.; Nazarov, R.; Neugebauer, J.: *Aspekte der Wasserstoffversprödung von Stählen: Verständnisgewinn durch quantenmechanische Simulationen.* (AKE Workshop, DECHEMA. Frankfurt a. M, Germany. 2013-10-24).

Hüter, C.: *Microstructure - Formation & Failure: Linking small scale wetting phenomena & mesoscale pattern formation processes* (TMS San Antonio, USA, 2013-03-06).

Jägle, E.: *Atom Probe Tomography: Basics, data analysis and application to the analysis of phase transformations.* (Colloquium at Max-Planck-Institute for Intelligent Systems. Stuttgart, Germany. 2013-01-28).

Kiener, D.; Oh, S. H.; Lee, S.; Jeong, J.; Minor, A. M.; Kunz, M.; Tamura, N.; Gruber, P. A.; Hoo, R. P.; Kirchlechner, C.; Alfreider, M.; Treml, R.: *In situ mechanical testing in electron microscopes to study small scale deformation mechanisms.* (ECI on Nanomechanical Testing 2013. Olhão (Algarve), Portugal. 2013-10-06 to 2013-10-11).

Kirchlechner, C.: *Insights into plastic deformation via X-ray μLaue diffraction.* (Summer School on: “Plasticity in small dimensions”. Cargese, France. 2013-10-14 to 2013-10-18).

Kirchlechner, C.: *In situ micromechanics: An overview on synchrotron based experiments.* (Seminar at KIT. Karlsruhe, Germany. 2013-04-24).

Kords, C.; Eisenlohr, P.; Roters, F.: *What contributes to the dislocation network stress driving continuum dislocation dynamics?* (Kolloquium der Forschergruppe 1650. Bad Herrenalb, Germany. 2013-05-03 to 2013-05-04).

Körmann, F.; Grabowski, B.; Dutta, B.; Hickel, T.; Neugebauer, J.: *First-Principles Thermodynamics of Paramagnetic Gama Fe.* (TMS Annual Meeting. San Antonio, TX, USA. 2013-03-04).

Mayrhofer, K. J. J.: Stability Investigations of Electrocatalysts for Electrochemical Energy Conversion. (Annual Symposium of the KNCV Working Group on Electrochemistry. Leiden, The Netherlands. 2013-11-29).

Mayrhofer, K. J. J.: *Kopplung von Elektrochemie mit zeitaufgelöster Elementanalytik.* (Jahrestagung 2013 der Gesellschaft für Korrosionsschutz e.V. Frankfurt/Main, Germany. 2013-11-12 to 2013-11-13).

Mayrhofer, K. J. J.: *Stability Investigations of Electrocatalysts for Electrochemical Energy Conversion.* (64th Annual Meeting of the International Society of Electrochemistry "Electrochemistry for a New Era". Santiago de Queretaro, Mexico. 2013-09-01 to 2013-09-13).

Mayrhofer, K. J. J.; Cherevko, S.; Topalov, A. A.; Žeradjanin, A. R.; Meier, J. C.; Schuppert, A. K.: *Stability of Noble Metal Catalysts for Electrochemical Energy Conversion.* (GDCH-Wissenschaftsforum 2013. Darmstadt, Germany. 2013-09-01 to 2013-09-04).

Mayrhofer, K. J. J.: *The particle-size effect in oxygen reduction electrochemistry on platinum - From model to real catalysts.* (Third Russian-German Conference on Catalysis "Bridging the Gap between Model and Real Catalysis. Energy-Related Catalysis". Lake Baikal, Russia. 2013-06-24 to 2013-06-27).

Mayrhofer, K. J. J.: *Stability of electrocatalysts on the nanoscale – Identical-location transmission electron microscopy.* (Insights from the Inside: Imaging Electrochemical Systems, Paul Scherrer Institut. Villigen, Switzerland. 2013-04-24).

Mayrhofer, K. J. J.: *Online-investigation of electrode material dissolution - Coupling electrochemistry to an ICP-MS.* (Deutsche Physikalische Gesellschaft Spring Meeting. Regensburg, Germany. 2013-03-11 to 2013-03-15).

Mayrhofer, K. J. J.: *Stability of electrocatalysts for electrochemical energy conversion.* (Seminar lecture at Carl-von-Ossietzky Universität Oldenburg, Germany. 2013-06-12).

Mayrhofer, K. J. J.: *Stability of Electrocatalysts for Electrochemical Energy Conversion.* (Seminar lecture at Ruhr-Universität Bochum, Germany. 2013-05-13).

Mayrhofer, K. J. J.: *Entwicklung einer Hochdurchsatzmethode gekoppelt mit in-situ Analytik für die Optimierung der elektrochemischen CO_2–Reduktion.* (Chemische Prozesse und Stoffliche Nutzung von CO_2 - 3. BMBF-Statuskonferenz - Seminar lecture. Berlin, Germany. 2013-04-10).

Millán, J.; Ponge, D.; Yuan, L.; Sandlöbes, S.; Goto, S.; Li, Y.; Choi, P.-P.; Zaefferer, S.; Nematollahi, G. A.; Herbig, M.; Kirchheim, R.; Inden, G.; Neugebauer, J.; Raabe, D.: *From defectant theory to nanoscale transformations in steels.* (Workshop on ‚Current Challenges in Materials Physics' at Physics Faculty, University Göttingen, Germany. 2013-05-24).

Millán, J.; Ponge, D.; Yuan, L.; Sandlöbes, S.; Goto, S.; Li, Y.; Choi, P.-P.; Zaefferer, S.; Nematollahi, G. A.; Herbig, M.; Kirchheim, R.; Inden, G.; Neugebauer, J.; Raabe, D.: *Nanoscale phase transformations at martensite interfaces.* (International Colloquium on Advanced Materials Simulation, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS). Bochum, Germany. 2013-05-06 to 2013-05-07).

Millán, J.; Ponge, D.; Povstugar, I.; Sandlöbes, S.; Choi, P.-P.; Zaefferer, S.; Haghighat, S. M. H.; Eggeler, G. F.; Nematollahi, G. A.; Herbig, M.; Kirchheim, R.; Inden, G.; Neugebauer, J.; Raabe, D.: *Scale-hoping approaches in desiging complex alloys.* (Royal Society International Seminar, Superalloys to Order' at the Kavli Royal Society International Centre. Chicheley, UK. 2013-04-22 to 2013-04-23).

Millán, J.; Ponge, D.; Yuan, L.; Sandlöbes, S.; Goto, S.; Li, Y.; Choi, P.; Zaefferer, S.; Nematollahi, A.; Herbig, M.; Kirchheim, R.; Neugebauer, J.; Raabe, D.: *Design of nanostructured bulk steels.* (Colloquium lecture at University of Bremen, Germany. 2013-04-30).

Motz, C.; Weygand, D.; Kirchlechner, C.; Zamanzade, M.; Tiba, I.; Berbenni, S.: *Plasticity in small dimensions and the influence of defect structure, boundaries and environment.* (ECI on Nanomechanical Testing 2013. Olhão (Algarve), Portugal. 2013-10-06 to 2013-10-11).

Neugebauer, J.: *Ab initio based free energy sampling.* (Workshop Talk. ESISM Workshop Kyoto, Japan. 2013-01-07 to 2013-01-09).

Neugebauer, J.: *Materials Design based on Predictive Ab Initio Thermodynamics.* (APS. Baltimore, MD, USA. 2013-03-18 to 2013-03-22).

Neugebauer, J.: *Computational coarse-graining in configuration space as basis for a predictive ab initio thermodynamics.* (EPSRC Symposium. Warwick, London, UK. 2013-12-09).

Neugebauer, J.: *Ab initio based multiscale modeling of structural materials: From a predictive thermodynamic description to tailored mechanical properties.* (CECAM Conference. Platja d'Aro, Spain. 2013-09-09 to 2013-09-13).

Neugebauer, J.: *Real Materials: Ab Initio Thermodynamics.* (Tutorial Workshop. Trieste, Italy. 2013-08-06 to 2013-08-08).

Neugebauer, J.: *Stahldesign in der Wunderwelt der Quantenmechanik.* (Tag der Offenen Tür, MPI für Eisenforschung GmbH. Düsseldorf, Germany. 2013-07-12).

Neugebauer, J.: *Vacancies in fcc metals: Discovery of large non-Arrhenius effects.* (German-Sino-Workshop. Bochum, Germany. 2013-06-17 to 2013-06-21).

Neugebauer, J.: Microstructure Control Based on *Ab Initio* Thermodynamics. (Workshop. Madrid, Spain. 2013-06-03 to 2013-06-03).

Neugebauer, J.: *Modeling Charged Defects and Impurities in a Thermodynamically Consistent Framework.* (Calphad Conference. San Sebastian, Spain. 2013-05-26 to 2013-05-31).

Neugebauer, J.: *Hydrogen embrittlement of metals: Novel approaches to an old.* (Colloquium at Universität Göttingen, Germany. 2013-05-24).

Neugebauer, J.: *Materials design based on predictive ab initio thermodynamics.* (ICAMS Colloquium. Bochum, Germany. 2013-05-06 to 2013-05-06).

Neugebauer, J.: *Understanding H-embrittlement in high-strength steels: An ab initio approach.* (CECAM Workshop. Lausanne, Switzerland. 2013-04-29 to 2013-05-02).

Neugebauer, J.: *Materials Design based on Predictive Ab Initio Thermodynamics.* (German-Sino-Workshop. Shenyang, China. 2013-04-13 to 2013-04-16).

Neugebauer, J.: *Fully ab initio determination of free energies: Basis for high-throughput approaches in materials design.* (DPG Frühjahrstagung 2013. Regensburg, Germany. 2013-03-11 to 2013-03-15).

Neugebauer, J.: *Smart microstructures by non-ergodic martensitic transitions.* (Non-ergodic behavior in martensites, Universität Duisburg-Essen. Duisburg, Germany. 2013-01-28 to 2013-01-30).

Neugebauer, J.: *Ab initio guided materials design: Application to doping and growth of group-III nitride.* (Colloquium, TH Ilmenau, Germany. 2013-01-17).

Neugebauer, J.: *Modeling steels exhibiting unconventional deformation mechanisms based on ab initio based multiscale simulations.* (ESISM Workshop. Kyoto, Japan. 2013-01-07 to 2013-01-09).

Neugebauer, J.: *Understanding and overcoming doping limits in GaN.* (SPIE Photonics West 2013. San Francisco, CA, USA. 2013-02-02 to 2013-02-07).

Palm, M.: *Current perspectives of iron aluminide based alloys.* (EUROMAT 2013. Sevilla, Spain. 2013-09-08 to 2013-09-13).

Ponge, D.; Millán, J.; Sandlöbes, S.; Choi, P.-P.; Hickel, T.; Kirchheim, R.; Neugebauer, J.; Raabe, D.: *Bulk Combinatorial Design of nanostructured steels: From composition to mechanisms.* (DPG Spring Meeting 2013. Regensburg, Germany. 2013-03-10 to 2013-03-15).

Prymak, O.; Enax, J.; Fabritius, H.-O.; Raabe, D.; Epple, M.: *Correlation of composition and structure of shark teeth.* (23rd Biomaterials in Medicine and Veterinary Medicine Conference. Rytro, Poland. 2013-10-09 to 2013-10-12).

Raabe, D.; Li, Y.; Ponge, D.; Sandlöbes, S.; Choi, P.-P.; Hickel, T.; Kirchheim, R.; Neugebauer, J.: *Nanoscale Transformations in Steels.* (German-Chinese High-level Workshop on "Microstructure-driven Design and Performance of Advanced Metals", Institute of Metals Research (IMR) of the Chinese Academy of Science (CAS). Shenyang, China. 2013-04-12 to 2013-04-16).

Raabe, D.; Li, Y.; Choi, P.-P.; Herbig, M.; Kirchheim, R.; Goto, S.: *Atomic-Scale Mechanisms of Strengthening in Wire Drawn Pearlite.* (MRS Fall Meeting. Boston, MA, USA. 2013-12-02).

Raabe, D.; Hickel, T.; Roters, F.; Neugebauer, J.: *Multiscale Modeling in Materials Science.* (Max Planck Society, LeadNet Meeting: 2013: Cross-sectional Workshop I: 'The Concept of Change', Castle Waldthausen. Mainz, Germany. 2013-05-06 to 2013-05-07).

Raabe, D.; Herbig, M.; Millán, J.; Ponge, D.; Li, Y.; Goto, S.; Sandlöbes, S.; Choi, P.; Kirchheim, R.; Neugebauer, J.: *Nanostructuring of bulk steels.* (International Conference on Computational Modeling of Nanostructured Materials - ICCMNM 2013, Frankfurt Institute for Advanced Studies. Frankfurt a. M.; Germany. 2013-09-03 to 2013-09-06).

Raabe, D.; Li, Y.; Ponge, D.; Sandlöbes, S.; Choi, P.; Hickel, T.; Kirchheim, R.; Neugebauer, J.: *Transformations in Steels.* (German-Chinese High-level Workshop on "Microstructure-driven Design and Performance of Advanced Metals", Institute of Metals Research (IMR) of the Chinese Academy of Science (CAS). Shenyang, China. 2013-04-14).

Raabe, D.; Ponge, D.; Goto, S.; Gutiérrez-Urrutia, I.; Choi, P.; Herbig, M.; Li, Y.; Zaefferer, S.; Kirchheim, R.: *Forget Spider Silk: Bulk Nanostructuring of 1 Billion Tons of Steel.* (Gordon Research Conference on Physical Metallurgy: Materials at Extremes, University of New England Biddeford. New England Biddeford, ME, USA. 2013-07-28 to 2013-08-02).

Raabe, D.; Choi, P.; Herbig, M.; Li, Y.; Zaefferer, S.; Kirchheim, R.: *Iron – Mythology and High Tech: From Electronic Understanding to Bulk Nanostructuring of 1 Billion Tons.* (Summer School 2013 on Functional Solids – FERRUM - organized by Leibniz University Hannover. Goslar, Germany. 2013-07-23).

Raabe, D.; Springer, H.; Eisenlohr, P.; Tasan, C. C.; Gutiérrez-Urrutia, I.; Choi, P.; Roters, F.; Zaefferer, S.; Koyama, N.; Kirchheim, R.; Li, Y.; Neugebauer, J.: *Nanostructuring 1 Billion Tons: Combining Rapid Alloy Prototyping, Multiscale Models, and Characterization for Advanced Manufacturing.* (2nd World Congress on Integrated Computational Materials Engineering. Salt Lake City, UT, USA. 2013-07-07 to 2013-07-11).

Rezaei Mianroodi, J.; Svendsen, B.: *Molecular Dynamics-Based Modeling of Dislocation-Stacking Fault Interaction.* (84th Annual Meeting of International Association of Applied Mathematics and Mechanics (GAMM). Novi Sad, Serbia. 2013-03-18 to 2013-03-22).

Rezaei Mianroodi, J.; Svendsen, B.: *Modeling and calculation of the stacking fault free energy of iron at high temperature.* (International Workshop Molecular Modeling and Simulation: Natural Science meets Engineering. Frankfurt a. M.; Germany. 2013-03-11 to 2013-03-12).

Rohwerder, M.: *Electrochemistry of metal surfaces under nanoscopic electrolyte layers.* (112th Bunsentagung (Annual German Conference on Physical Chemistry). Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany. 2013-05-09 to 2013-05-11).

Rohwerder, M.: *Selbstheilung metallischer Überzüge durch Einbau Inhibitor-beladener Silicapartikel.* (708. DECHEMA-Kolloquium. Frankfurt a. M.; Germany. 2013-03-14).

Rohwerder, M.: *Neuartige intelligent selbstheilende Korrosionsschutzsysteme.* (5. Korrosionsschutz-Symposium, Korrosionsschutz durch Beschichtungen in Theorie und Praxis. Kloster Banz, Germany. 2013-06-12 to 2013-06-14).

Roters, F.; Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Raabe, D.: *A spectral method solution to crystal elasto-viscoplasticity at finite strains.* ("Textures, Microstructures and Plastic Anisotropy, a Tribute to Paul Van Houtte". KU Leuven, Belgium. 2013-03-14 to 2013-03-15).

Roters, F.: *Modellierung von Verformungsvorgängen auf Basis der Kristallplastizität.* (Herbstschule des SFB 799 TRIP-Matrix-Composite. Leipzig, Germany. 2013-09-02).

Roters, F.; Eisenlohr, P.; Diehl, M.; Shanthraj, P.; Kords, C.; Raabe, D.: *Das flexible Kristalplastizitäts-Modell 'DAMASK'.* (Semniar at Lehrstuhl für Werkstoffkunde und Werkstoffmechanik, Technische Universität München. Garching, Germany. 2013-07-03).

Roters, F.; Eisenlohr, P.; Diehl, M.; Shanthraj, P.; Kords, C.; Raabe, D.: *The general crystal plasticity framework 'DAMASK'.* (Seminar at Institute of Materials Simulation, Department of Materials Science, University of Erlangen-Nürnberg. Fürth, Germany. 2013-06-12).

Roters, F.; Diehl, M.; Shanthraj, P.; Lebensohn, R. A.; Eisenlohr, P.: *A spectral method solution to crystal elastoviscoplasticity at finite strains.* (Plasticity '13, The 19th International Symposium on Plasticity & Its Current Applications. Nassau, Bahamas. 2013-01-03 to 2013-01-08).

Shanthraj, P.; Diehl, M.; Eisenlohr, P.; Roters, F.: *Advanced spectral methods to study mechanics of heterogeneous materials.* (SPP1420 PhD and PostDoc workshop. Darmstadt, Germany. 2013-06-17 to 2013-06-18).

Springer, H.; Belde, M.; Raabe, D.: *Examples of novel steel design: Ductile high strength martensitic steels developed by combinatorial techniques and liquid metallurgy MMCs with high stiffness and low density.* (Workshop "new frontiers in steel design", Institut für neue Materialien, Universität Saarbrücken, Germany. 2013-11-12).

Springer, H.; Raabe, D.: *Effizientes Legierungsdesign durch kombinatorische Metallurgie und Prozesstechnik.* (Forschungsdialog Rheinland, IHK Wuppertal-Solingen-Remscheid. Wuppertal, Germany. 2013-07-03).

Springer, H.; Raabe, D.: *Rapid Alloy Prototyping - Effizientes Legierungsdesign durch kombinatorische Metallurgie und Prozesstechnik.* (Seminar at RWTH Aachen MCh. Aachen, Germany. 2013-01-30).

Stein, F.: *Experiments on the Peritectoid Decomposition Kinetics of the Intermetallic Phase Nb_2Co_7.* (4th Sino-German Symposium on Computational Thermodynamics and Kinetics and Its Application to Materials Processing. Bochum, Germany. 2013-06-17 to 2013-06-21).

Stein, F.: *Stability, Structure and Mechanical Properties of Transition-Metal-Based Laves Phases.* (Institut de Chimie et des Matériaux, CNRS-Université Paris Est. Paris, France. 2013-06-25).

Stein, F.; Li, X.; Scherf, A.; Janda, D.; Heilmaier, M.: *Al-rich Fe–Al: An in situ Composite Material with Fine-Scaled, Lamellar Microstructure.* (Thermec 2013. Las Vegas, NV, USA. 2013-12-02 to 2013-12-06).

Stoffers, A.; Cojocaru-Mirédin, O.; Breitenstein, O.; Seifert, W.; Raabe, D.: *Recombination activity at the atomic scale: Correlative analysis of grain boundaries in multicrystalline silicon solar cells.* (Euromat 2013. Sevilla, Spain. 2013-09-08 to 2013-09-13).

Svendsen, B.: *Phase-field modeling of dislocation transport.* (A Conference Celebrating the 70th Birthday of Thomas J.R. Hughes. San Diego, CA, USA. 2013-02-24 to 2013-02-27).

Tasan, C. C.: *Micro/nano-mechanical analysis of novel multi-phase alloys.* (Karlsruhe Institute of Technology. Karlsruhe, Germany. 2013-11-27).

Todorova, M.; Neugebauer, J.: *Extending the Concept of Semiconductor Defect Chemistry to Electrochemistry.* (TMS Annual Meeting. San Antonio, TX, USA. 2013-03-03 to 2013-03-07).

Vogel, S. C.; Brown, D. W.; Okuniewski, M.; Stebner, A.; Stein, F.: *Characterization of Intermetallics with the HIPPO & SMARTS Neutron Beam-Lines at LANSCE.* (Intermetallics 2013, Educational Center Kloster Banz. Bad Staffelstein, Germany. 2013-09-30 to 2013-10-04).

Wippermann, S. M.; Vörös, M.; Rocca, D.; Li, T.; Gali, A.; Zimanyi, G. T.; Galli, G.: *Semiconducting Nano-Composites for Solar Energy Conversion: Insights from ab initio calculations.* (CECAM Workshop CPMD-2013. Leipzig, Germany. 2013-09-02 to 2013-09-06).

Yan, D.; Tasan, C. C.; Raabe, D.: *High resolution strain mapping coupled with EBSD during in-situ tension in SEM.* (Interdisciplinary Center for Advanced materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany. 2013-09-20).

Zaefferer, S.; Elhami, N. N.; Konijnenberg, P. J.; Jäpel, T.: *Quantitative Microstructure Characterization by Application of Advanced SEM-Based Electron Diffraction Techniques.* (Microscopy and Microanalysis 2013. Indianapolis, IN, USA. 2013-08-04 to 2013-08-08).

Zaefferer, S.: *An overview on techniques for high spatial resolution measurements of plastic and elastic strain by EBSD and related techniques.* (RexGG pre-conference workshop. Wollongong, Australia. 2013-05-06).

Zaefferer, S.: *An overview on techniques for high spatial resolution measurements of plastic and elastic strain by EBSD and related techniques.* (MicroCar 2013. Leipzig, Germany. 2013-02-25 to 2013-02-26).

Zaefferer, S.: *Accurate and quantitative measurement of plastic strain by SEM-based diffraction techniques.* (RexGG 2013. Sydney, Australia. 2013-05-05 to 2013-05-10).

Zaefferer, S.: Observation of dislocation evolution during in-situ nano indentation using electron channelling contrast imaging (ECCI). (Kleindiek Usermeeting 2013. Kusterdingen, Germany. 2013-04-16).

Žeradjanin, A. R.: *Impact of the spatial distribution of morphological patterns on the efficiency of electrocatalytic gas evolving reactions.* (Seminar at Serbian Chemical Society. Belgrade, Serbia. 2013-05-09).

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Balila, N. J.; Kirchlechner, C.; Dehm, G.: *Design and development of fracture property measurement techniques at the small scale*. (ICAMS (RUB). Bochum, Germany. 2014-04-14).

Choi, P.-P.: *Characterization of Ni- and Co-based superalloys using Atom Probe Tomography*. (International Workshop on Modelling and Simulation of Superalloys. Bochum, Germany. 2014-09-15 to 2014-09-17).

Cojocaru-Mirédin, O.; Soni, P. U.; Würz, R.; Raabe, D.: *Progress in interfaces characterization in solar cells using correlative techniques*. (Atom Probe Tomography & Microscopy 2014. Stuttgart, Germany. 2014-08-31 to 2014-09-05).

Cojocaru-Mirédin, O.; Choi, P.-P.; Abou-Ras, D.; Würz, R.; Sáez-Araoz, R.; Fischer, C.-H.; Raabe, D.: *Characterization of internal interfaces in Cu(In,Ga)Se_2 thin-film solar cells using correlative microscopies*. (40th PVSC IEEE 2014. Denver, CO, USA. 2014-06-08 to 2014-06-13).

Cojocaru-Mirédin, O.; Stoffers, A.; Soni, P. U.; Würz, R.; Raabe, D.: *Interfaces in Semiconductors: Application to photovoltaic materials*. (61st American Vacuum Society International conference. Baltimore, MA, USA. 2014-11-09 to 2014-11-14).

Dehm, G.: *Plasticity of supersaturated Cu–Cr alloys and Cu–Cr multilayers*. (MACAN Meeting. Düsseldorf, Germany. 2014-06-30 to 2014-07-02).

Dehm, G.: *Cu–Cr nanocomposites and multilayers*. (Gordon Research Conference: Thin Film & Small Scale Mechanical Behavior. Bentley University, Boston, MA, USA. 2014-07-13 to 2014-07-18).

Dehm, G.: *In situ Transmission Electron Microscopy*. (GRK 1896 Summer School on In situ Microscopy. Hirschegg, Austria. 2014-09-21 to 2014-09-25).

Dehm, G.: *Localized mechanical study of individual interfaces in miniaturized Cu structures*. (MS&T14 - Materials Science & Technology 2014. Pittsburgh, PA, USA. 2014-10-12 to 2014-10-16).

Dehm, G.: *Small Scale Mechanical Testing: More than just a fashionably tool?!* (Kolloquium für Mechanik, KIT. Karlsruhe, Germany. 2014-11-20 to 2014-11-20).

Dehm, G.: *Differences in deformation behavior of Cu structures containing individual grain boundaries*. (Symposium RR: Scaling Effects in Plasticity - Synergy between Simulations and Experiments, Fall MRS. Boston, MA, USA. 2014-11-30 to 2014-12-05).

Dehm, G.: *From idealized bi-crystals towards applied polycrystals: Plastic deformation in small dimensions*. (Schöntal Symposium - Dislocation-based Plasticity. Kloster Schöntal, Germany. 2014-02-24 to 2014-02-28).

Dehm, G.; Imrich, P. J.; Wimmer, A. C.; Kirchlechner, C.: *From idealized bi-crystals towards applied polycrystals: Plastic deformation in small dimensions*. (TMS2014, 143rd Annual Meeting & Exhibition. San Diego, CA, USA. 2014-02-16 to 2014-02-20).

Dutta, B.; Hickel, T.; Neugebauer, J.: *Coupling of lattice dynamics and magnetism in magnetic shape memory alloys: Consequences for phase diagrams*. (Asia Sweden meeting on understanding functional materials from lattice dynamics (ASMFLD) conference. Indian Institute of technology Guwahati, India. 2014-01-09 to 2014-01-11).

Enax, J.; Fabritius, H.-O.; Prymak, O.; Raabe, D.; Epple, M.: *Synthetic dental composite materials inspired by shark teeth*. (Annual Meeting of the Canadian Biomaterials Society. Halifax, Nova Scotia, Canada. 2014-06-04 to 2014-06-07).

Enax, J.; Fabritius, H.-O.; Roters, F.; Raabe, D.; Epple, M.: *Synthetic dental composite materials inspired by the hierarchical organization of shark tooth enameloid*. (Third winter school within the DFG priority programme 1420 "Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials". Potsdam, Germany. 2014-03-17 to 2014-03-18).

Fabritius, H.-O.: *Biological Photonic Structures*. (Keynote at the Kick-Off meeting of the DFG SPP1839, Wilhelm-Conrad-Roentgen Campus (Bessy II). Berlin, Germany. 2014-09-25).

Fabritius, H.-O.: *Structure-property relations in biological composite materials*. (Seminar at Department of Earth- and Environmental Sciences, LMU München, Germany. 2014-02-21).

Fabritius, H.-O.: *Structure-property relations in biological composite materials – The arthropod exoskeleton*. (Chemical Engineering and Materials Science Seminar, Michigan State University. East Lensing, MI, USA. 2014-10-09).

Fabritius, H.-O.; Janus, A. M.; Wu, X.; Nikolov, S.; Eisenlohr, P.; Friák, M.; Neugebauer, J.; Raabe, D.: *Structure-property Relations in the Arthropod Exoskeleton, a Multifunctional Biological Composite*. (Materials Science & Technology (MS&T) 2014. Pittsburgh, PA, USA. 2014-10-12 to 2014-10-16).

Freysoldt, C.: *Die S/PHI/nX-Klassenbibliothek - HPC-Programmierung für Physiker*. (Workshop „High-performance computing und datengetriebene Anwendungen in der MPG. Ringberg, Germany. 2014-02-05 to 2014-02-07).

Freysoldt, C.; Pfanner, G.; Neugebauer, J.: *Role of the defect creation strategy for modelling dangling bonds in a-Si:H*. (MRS Spring Meeting. San Francisco, CA, USA. 2014-04-21 to 2014-04-25).

Freysoldt, C.; Neugebauer, J.: *Point defects in supercells: Correction schemes for the dilute limit*. (Workshop on Ab-initio description of charged systems and solid/liquid interfaces. Santa Barbara, CA, USA. 2014-07-07 to 2014-07-11).

Gutiérrez-Urrutia, I.; Raabe, D.: *Exploring nanotwinned structures in advanced high-Mn steels*. (International Symposium on Plasticity 2014. Freeport, BS, USA. 2014-01-03 to 2014-01-08).

Haghighat, S. M. H.; Raabe, D.; von Pezold, J.; Race, C. P.; Körmann, F.; Friák, M.; Schäublin, R.; Neugebauer, J.; Eggeler, G. F.: *Recent development of modelling techniques in nano- and meso-scale simulations of dislocation dynamics*. (Workshop on Integrated Computational Materials Engineering (ICME). Rolduc Abbey, The Netherlands. 2014-06-24 to 2014-06-27).

Haghighat, S. M. H.; Li, Z.; Zaefferer, S.; Reed, R.; Raabe, D.: *Mesoscale modeling of dislocation climb and primary creep process in single crystal Ni base superalloys*. (International Workshop on Dislocation Dynamics Simulations. Saclay, France. 2014-12-10 to 2014-12-12).

Haghighat, S. M. H.; Eggeler, G. F.; Raabe, D.: *Mesoscale modelling of the influence of loading conditions on the dislocation mobility and creep process in single crystal Ni base superalloys*. (KTH Royal Institute of Technology. Stockholm, Sweden. 2014-04-24).

Herbig, M.: *Joint Characterization of Crystallography and Chemistry on the Nanometer Scale by Correlative Electron Microscopy and Atom Probe Tomography*. (Seminar talk at the Institut für Metallkunde und Metallphysik, RWTH Aachen, Germany. 2014-10-21).

Herbig, M.; Li, Y.; Morsdorf, L.; Goto, S.; Choi, P.-P.; Kirchheim, R.; Raabe, D.: *Bulk Nanostructured Steels*. (Seminar at Ecole Polytechnique Federale de Lausanne (EPFL), Institute of Materials (IMX). Lausanne, France. 2014-11-17).

Herbig, M.; Choi, P.-P.; Raabe, D.: *Atom Probe Tomography and Correlative TEM/APT at the MPIE*. (Mini-Symposium Atom Probe Tomography, National APT Facility Eindhoven, TU Delft, The Netherlands. 2014-05-27).

Herbig, M.; Kim, J.-H.; Ponge, D.; Li, Y.; Morsdorf, L.; Goto, S.; Haley, D.; Koyama, M.; Bashir, A.; Merzlikin, S. V.; Rohwerder, M.; Akiyama, E.; Tsuzaki, K.; Kuzmina, M.; Sandlöbes, S.; Choi, P.-P.; Kirchheim, R.; Raabe, D.: *Nanostructure Manipulation by Segregation Engineering*. (2nd ESISM International Workshop on Fundamental Issues of Structural Materials. Kyoto, Japan. 2014-03-11 to 2014-03-12).

Herbig, M.; Li, Y.; Morsdorf, L.; Goto, S.; Choi, P.-P.; Kirchheim, R.; Raabe, D.: *Nanostructure Manipulation by Segregation Engineering*. (George Smith Symposium on Atom Probe Tomography. Oxford, UK. 2014-04-07 to 2014-04-09).

Herbig, M.; Li, Y.; Morsdorf, L.; Goto, S.; Choi, P.-P.; Kirchheim, R.; Raabe, D.: *Recent Advances in Understanding the Structures and Properties of Nanomaterials*. (Gordon Research Conference on Structural Nanomaterials, The Chinese University of Hong Kong, China. 2014-07-20 to 2014-07-25).

Herbig, M.; Choi, P.; Raabe, D.: *Atom Probe Tomography and Correlative TEM/APT at the MPIE*. (Inauguration of the Atom Probe at the Institute for Physics IA at the RWTH Aachen, Germany. 2014-03-17).

Hickel, T.; Glensk, A.; Grabowski, B.; Körmann, F.; Neugebauer, J.: *Thermodynamics of materials up to the melting point: The role of anharmonicities*. (Asia Sweden Meeting on Understanding Functional Materials from Lattice dynamics. Guwahati, India. 2014-01-09 to 2014-01-11).

Hickel, T.; Nazarov, R.; McEniry, E.; Chakrabarty, A.; Dey, P.; Aydin, U.; Leyson, G.; Grabowski, B.; Neugebauer, J.: *Ab initio based understanding of the segregation and diffusion mechanisms of hydrogen in steels*. (Workshop on Hydrogen Embrittlement. Düsseldorf, Germany. 2014-01-23).

Hickel, T.; Nazarov, R.; McEniry, E.; Chakrabarty, A.; Dey, P.; Spatschek, R. P.; Grabowski, B.; Neugebauer, J.: *Ab initio based understanding of the segregation and diffusion mechanisms of hydrogen in steels*. (TMS Annual Meeting 2014. San Diego, CA, USA. 2014-02-16 to 2014-02-20).

Hickel, T.; Nazarov, R.; McEniry, E.; Chakrabarty, A.; Dey, P.; Aydin, U.; Leyson, G.; Grabowski, B.; Neugebauer, J.: *Ab initio based understanding of the segregation and diffusion mechanisms of hydrogen in steels*. (SteelyHydrogen 2014, International conference on hydrogen in steels. Ghent, Belgium. 2014-05-05 to 2014-05-07).

Hickel, T.; Körmann, F.; Bleskov, I.; Neugebauer, J.: *Ab Initio Based Modelling of Stacking Fault Energies in High-Strength Steels*. (International Seminar on Process Chain Simulation and Related Topics. Karlsruhe, Germany. 2014-03-17 to 2014-03-19).

Hickel, T.: *Understanding complex materials at finite temperatures by ab inito methods*. (Physikalisches Kolloquium der TU Chemnitz, Germany. 2014-04-16).

Hickel, T.: *Understanding complex materials at finite temperatures by ab inito methods*. (Colloquium at Institut für Materialwissenschaft, Universtität Stuttgart, Germany. 2014-11-24).

Hickel, T.: *Ab initio basierte Methoden der mechanismen-orientierten Werkstoffentwicklung*. (Colloquium at Salzgitter-Mannesmann-Forschung GmbH. Duisburg, Germany. 2014-05-08).

Hickel, T.; Nazarov, R.; McEniry, E.; Dey, P.; Neugebauer, J.: *Impact of light elements on interface properties in steels*. (CECAM workshop “Modeling Metal Failure Across Multiple Scales”. Lausanne, Switzerland. 2014-05-26 to 2014-05-27).

Hickel, T.; Glensk, A.; Nazarov, R.; Sözen, H. I.; Grabowski, B.; Neugebauer, J.: *Ab initio determination of point defects and derived diffusion properties in metals*. (International conference on diffusion in materials, DIMAT2014. Münster, Germany. 2014-08-17 to 2014-08-22).

Imrich, P. J.; Kirchlechner, C.; Motz, C.; Jeon, J. B.; Dehm, G.: *In Situ Electron Microscopy and Micro-Laue Study of Plasticity in Miniaturized Cu Bicrystals*. (CAMTEC III, Symposium on Fine-Scale Mechanical Characterisation and Behaviour. Cambridge, UK. 2014-04-07 to 2014-04-08).

Kirchlechner, C.; Motz, C.; Imrich, P. J.; Dehm, G.: *A novel view on fatigue damage at the micron scale by in situ X-ray µLaue diffraction*. (TMS2014. San Diego, CA, USA. 2014-02-16 to 2014-02-20).

Kirchlechner, C.: *New insights into the plasticity of micron sized objects by in situ µLaue diffraction*. (Lecture at Universität Münster, Germany. 2014-07-11).

Kirchlechner, C.: *From Idealized Single Crystals Towards Applied Polycrystals: Insights by X-Ray µLaue Diffraction*. (The Thin Film & Small Scale Mechanical Behavior - Gordon Research Conference (GRC). Waltham, MA, USA. 2014-07-13 to 2014-07-18).

Kirchlechner, C.: *“What can we learn from X-ray µLaue diffraction and where do we need to be careful?”*. (Seminar Talk at Helmholtz-Zentrum Geesthacht, Germany. 2014-11-27).

Kirchlechner, C.: *In situ micromechanics: An overview on synchrotron based µLaue experiments*. (XTOP 2014. Villard de Lans, France. 2014-09-17).

Konijnenberg, P. J.; Stechmann, G.; Zaefferer, S.; Raabe, D.: *Advances in Analysis of 3D Orientation Data Sets Obtained by FIB-EBSD Tomography*. (2nd International Congress on 3D Materials Science 2014. Annecy, France. 2014-06-29 to 2014-07-02).

Körmann, F.; Hickel, T.; Neugebauer, J.: *Phase stabilities of metals and steels - The impact of magnetic excitations from fi rst-principles*. (ADIS (Ab initio Description of Iron and Steel) Conference 2014. Ringberg Castle, Rottach-Egern, Germany. 2014-10-27).

Mayrhofer, K. J. J.: *Scanning Electrochemical Microscopy: Reading, Writing, Monitoring of Functional Interfaces*. (65th Annual Meeting of the International Society of Electrochemistry, Symposium. Lausanne, Switzerland. 2014-08-31 to 2014-09-05).

Mayrhofer, K. J. J.: *Basic Science and Key Technologies for Future Applications*. (Electrochemistry 2014, Johannes Gutentenberg-Universität Mainz, Germany. 2014-09-22 to 2014-09-24).

Mayrhofer, K. J. J.: *Combinatorial study of fundamental electrocatalyst performance of materials for oxygen evolution*. (Heraeus seminar “From Sunlight to Fuels - Novel Materials and Processes for Photovoltaic and (Photo)Catalytic Applications”. Bad Honnef, Germany. 2014-05-11 to 2014-05-16).

Mayrhofer, K. J. J.: *Oxygen electrochemistry as a cornerstone for sustainable energy conversion*. (International Symposium „Recent Achievements and Future Trends in Electrocatalysis“. Erlangen, Germany. 2014-04-04).

Mayrhofer, K. J. J.: *Stability of catalyst materials - the key for the deployment of electrochemical energy conversion*. (Seminar lecture at Gesellschaft Deutscher Chemiker. Mülheim/Ruhr, Germany. 2014-01-10).

Mayrhofer, K. J. J.: *Electrochemical Energy Conversion – The key for sustainable utilization of solar energy*. (Pregl Seminar lecture, National Institute of Chemistry. Ljubljana, Slovenia. 2014-10-23).

Mayrhofer, K. J. J.: *Stability Investigations of Electrocatalysts for Electrochemical Energy Conversion*. (Seminar lecture at Helmholtz-Zentrum Berlin, Germany. 2014-07-03).

Neugebauer, J.: *Interplay between Plasticity Mechanisms, Entropy, and Chemical Composition: An Ab initio approach*. (Plasticity 2014. Freeport, Bahamas. 2014-01-03 to 2014-01-08).

Neugebauer, J.: *Materials design and discovery on the computer: Prospects and challenges*. (ICYS workshop. Tsukuba, Japan. 2014-01-13 to 2014-01-15).

Neugebauer, J.: *Ab initio thermodynamics: A novel route to understand and design structural materials*. (NIMS. Tsukuba, Japan. 2014-01-15 to 2014-01-17).

Neugebauer, J.: *Materials design based on predictive ab initio thermodynamics*. (Colloquium at Universität Magdeburg, Germany. 2014-01-28).

Neugebauer, J.: *A brief introduction to surface science from a modelers perspective*. (Seminar at Ecole Polytechnique. Paris, France. 2014-03-11).

Neugebauer, J.: *Pourbaix diagrams and stability in electrochemical environment*. (Catalysis Workshop Reisensburg, Germany. 2014-05-25 to 2014-05-28).

Neugebauer, J.: *Connecting thermodynamic concepts of semiconductor defect chemistry with electrochemistry.* (Calphad Conference. Changsha, China. 2013-06-02 to 2013-06-06).

Neugebauer, J.: *Understanding hydrogen embrittlement by a combined atomistic-analytic multiscale approach*. (MDRC Conference. Lake Arrowhead, CA, USA. 2014-06-08 to 2014-06-13).

Neugebauer, J.: *Discrete Models – Material Properties from Electrons and Atoms*. (ICMEg Conference. Rolduc, The Netherlands. 2014-06-24 to 2014-06-27).

Neugebauer, J.: *Efficient coarse graining of stochastic high-dimensional configuration spaces as fundament for a fully ab initio based materials design*. (Colloquium WIAS. Berlin, Germany. 2014-06-30).

Neugebauer, J.: *First principles calculations of CCA stability*. (Workshop CC Alloys. München, Germany. 2014-07-15 to 2014-07-18).

Neugebauer, J.: *Ab initio thermodynamics: A novel route to understand and design structural materials*. (CSW Conference. Tsukuba, Japan. 2014-08-20 to 2014-08-22).

Neugebauer, J.: *Materials design and discovery on the computer: Prospects and challenges*. (IUMRS-ICA2014. Fukuoka, Japan. 2014-08-20 to 2014-08-22).

Neugebauer, J.: *Materials design based on predictive ab initio thermodynamics*. (CMD25 JMC. Paris, France. 2014-08-24 to 2014-08-29).

Neugebauer, J.: *Modeling Ductility at the Atomistic Scale: Status and Challenges*. (MSE 2014. Darmstadt, Germany. 2014-09-23 to 2014-09-25).

Neugebauer, J.: *The role of hydrogen-hydrogen interaction in understanding H embrittlement: An ab initio guided multiscale approach*. (Hydrogen Conference. London, UK. 2014-10-16 to 2014-10-18).

Neugebauer, J.: *Design of structural materials based on ab initio computed phase stabilities*. (MS&T Conference. Orlando, FL, USA. 2014-10-12 to 2014-10-16).

Neugebauer, J.: *Ab initio based design of structural materials: Status and challenges*. (Expertenpanel Computer Simulation of Material Structures and Properties, Schott AG. Mainz, Germany. 2014-11-14).

Neugebauer, J.: *Identifying H induced failure mechanisms in structural materials: A multiscale approach*. (MRS Fall Meeting. Boston, MA, USA. 2014-11-30 to 2014-12-05).

Palm, M.: *Alloy development and industrial processing of iron aluminide based alloys*. (Czech-Japanese Workshop on High-Temperature Intermetallics. Brno, Czech Republic. 2014-04-13 to 2014-04-16).

Palm, M.: *Alloy development and industrial processing of iron aluminide based alloys*. (IMDEA 2014 - Seminar Series. Getafe, Spain. 2014-05-26 to 2014-05-26).

Raabe, D.; Ponge, D.; Gutiérrez-Urrutia, I.; Springer, H.; Kuzmina, M.; Hickel, T.; Welsch, E.; Haghighat, S. M. H.; Sandlöbes, S.; Choi, P.-P.; Neugebauer, J.: *Designing bulk nanostructured high manganese steels by intregrating advanced characteriation and ab initio modeling*. (2nd International Conference on High Manganese Steels - HMnS 2014. Aachen, Germany. 2014-08-31 to 2014-09-04).

Ram, F.; Zaefferer, S.: *Accurate Kikuchi band localization and its application for diffraction geometry determination*. (HR-EBSD workshop, Imperial College. London, UK. 2014-04).

Rohwerder, M.: *Scanning Kelvin Probe Force Microscopy as Tool for the Investigation of Localized Corrosion*. (2014 ECS and SMEQ Joint Internat. Meeting. Cancun, Mexico. 2014-10-05 to 2014-10-09).

Rohwerder, M.: *Selbstheilende Beschichtungen für den Korrosionsschutz: Ein kritischer Überblick*. (28. Sitzung des AK "Korrosionsschutz durch Beschichtungen", GfKorr. Frankfurt, Germany. 2014-11-06).

Rohwerder, M.: *Self-Healing Coatings for Corrosion Protection: A Critical Overview and Latest Results*. (BASF Corrosion Workshop. Ludwigshafen, Germany. 2014-10-01).

Rohwerder, M.: *General corrosion mechanisms: Protection by organic coatings and novel intelligent pigments*. (Axalta Innovation Symposium. Düsseldorf, Germany. 2014-09-10).

Rohwerder, M.: *Self-Healing Coatings for Corrosion Protection: A Critical Overview and Latest Results*. (Gordon Reserach Conference on Aqueous Corrosion. New London, AR, USA. 2014-07-13 to 2014-07-18).

Rohwerder, M.: *Korrosionsschutz mit leitfähigen Polymeren: Entwicklung selbstheilender Beschichtungen*. (Materials Valley Workshop. Hanau, Germany. 2014-03-13).

Rohwerder, M.: *Zinc alloy coatings for corrosion protection: From the basics to new challenges*. (MSE Colloquium, The Ohio State University, Columbus, OH, USA. 2014-02-10).

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Dehm, G.: *Small Scale Mechanical Testing: More than just a fashionably tool?!* (POSTECH. Pohang, South-Korea. 2015-03-12).

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Grabowski, B.: *Atomistic origin of superior mechanical properties of Gum Metals* (ICCP9, Singapore, 2015-01).

Grabowski, B.: *Auf dem Weg zu selbstheilenden Stählen: Herausforderungen und potenzielle Strategien* (Stahlmarkt, Düsseldorf, 2015-02).

Grabowski, B.: *Origin of anharmonicity in fcc materials* (Seminar at KTH Stockholm, Sweden, 2015-03).

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Mayrhofer, K. J. J.: *Novel in situ in operando methods.* (66th meeting of the International Society of Electrochemistry, Symposium "Novel in situ in operando methods". Taipei, Taiwan. 2015-10-04 to 2015-10-09).

Mayrhofer, K. J. J.: *Combinatorial screening of catalyst materials for electrochemical CO_2 reduction.* (ACHEMA 2015, Industrial carbon dioxide utilization. Frankfurt, Germany. 2015-06-15 to 2015-06-19).

Mayrhofer, K. J. J.: *Combinatorial study of fundamental electrocatalyst performance - The Scanning Flow Cell coupled to online analytics.* (227th annual meeting of the Electrochemical Society, Symposium "State-of-the-Art Tutorial on Diagnostics in Low-Temperature Fuel Cells". Chicago, IL, USA. 2015-05-24 to 2015-05-28).

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Mayrhofer, K. J. J.: *Time and potential resolved dissolution of Pt and Au.* (Catalysis for solar fuels – Fundamentals and application - Workshop lecture at Technical University München, Germany. 2015-02-27).

Mayrhofer, K. J. J.: *Corrosion of electrocatalysts – An essential avenue towards efficient electrochemical energy conversion.* (Crossroads in electrochemistry - Symposium lecture at Fritz-Haber-Institut der MPG. Berlin, Germany. 2015-01-14 to 2015-01-15).

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Neugebauer, J.: *Big Data im computergestützten Materialdesign.* (CPTS Big Data round table. Tübingen, Germany. 2015-01-26 to 2015-01-27).

Neugebauer, J.: *Quantum mechanical design of structural materials on the computer.* (Colloquium at Heinrich Heine Universität Düsseldorf, Germany. 2015-02-02).

Neugebauer, J.: *Ab Initio Thermodynamics: A Novel Route to Design Structural Materials with Superior Mechanical Properties.* (TMS-MEMA Conference. Doha, Katar. 2015-01-11 to 2015-01-14).

Neugebauer, J.: *A brief introduction to surface science from a modelers perspective.* (Colloquium at Ecole Polytechnique. Paris, France. 2015-02-10).

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Neugebauer, J.: *Multi scale Simulation of complex materials under realistic environments.* (RESOLV Workshop. Velen, Germany. 2015-03-09 to 2015-03-11).

Neugebauer, J.: *Materials design based on predictive ab initio thermodynamics.* (Colloquium at Lawrence Livermore National Lab. Livermore, CA, USA. 2015-04-13).

Neugebauer, J.: *Ab initio description of finite temperature phase stabilities and transformations.* (PTM Conference. Whistler, Canada. 2015-06-28 to 2015-07-03).

Neugebauer, J.: *Ab initio thermodynamics: A novel route to design materials on the computer.* (Colloquium at Universität Marburg, Germany. 2015-05-07).

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Neugebauer, J.: *Electrochemistry from a semiconductor physics perspective: New tools and insights.* (SurMat Workshop. Düsseldorf, Germany. 2015-04-27).

Neugebauer, J.: *From surface modeling to novel semiconductor growth strategies.* (MDRC Conference on Material Defects. Lake Arrowhead, CA, USA. 2015-06-07 to 2015-06-12).

Neugebauer, J.: *Ordering phenomena in InGaN.* (Lecture at University of California, Santa Barbara, CA, USA. 2015-04-16 to 2015-04-16).

Neugebauer, J.: *Overcoming Growth Limitations by ab initio Guided Surface Engineering.* (ICMCTF Conference. San Diego, CA, USA. 2015-04-20 to 2015-04-25).

Neugebauer, J.: *Point Defects at Finite Temperatures.* (Conference and Workshop "Nothing is perfect. Monte Verita, Switzerland. 2015-04-26 to 2015-04-29).

Neugebauer, J.: *Pylron – A Python Based Workbench for Automated Atomistic Simulations.* (CECAM Conference. Lausanne, Switzerland. 2015-06-08 to 2015-06-10).

Neugebauer, J.: *Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach.* (International Workshop MoD-PMI. Marseille, France. 2015-05-25 to 2015-05-27).

Neugebauer, J.: *Design of structural materials by ab initio guided multiscale simulations.* (CMRI Symposium. Sendai, Japan. 2015-10-13 to 2015-10-14).

Neugebauer, J.: *Towards automated toolsets for computing high-precision free energies by ab initio approaches.* (MS&T. Columbus, OH, USA. 2015-10-04 to 2015-10-08).

Neugebauer, J.: *Design of structural materials by predictive ab initio thermodynamics: Challenges, applications and perspectives.* (Euromat Conference. Warsaw, Poland. 2015-09-20 to 2015-09-24).

Neugebauer, J.: *Ab Initio Computation of Phonon-Phonon and Magnon-Phonon Interactions: Successes and Challenges.* (Workshop DyProSo. Freising, Germany. 2015-09-13 to 2015-09-17).

Neugebauer, J.: *Ab initio guided design of structurally and thermodynamically complex materials.* (Psi-k 2015 Conference. San Sebastian, Spain. 2015-09-08 to 2015-09-10).

Neugebauer, J.: *Quantum-mechanical approaches to address the structural and thermodynamic complexity of engineering materials.* (Swedish Chemical Society. Kalmar, Sweden. 2015-08-23 to 2015-08-28).

Neugebauer, J.: *Vacancies in fcc metals: Discovery of large non-Arrhenius effects.* (The 5th Sino-German Symposium Thermodynamics and Kinetics of Nano and Mesoscale Materials and Their Applications. Changchun, China. 2015-07-26 to 2015-07-31).

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Doctoral, Diploma, Master and Bachelor Theses

Doctoral Theses

2012 (not included in Scientific Report 2011-2012)

Dr.-Ing. C. Begau: Characterization of crystal defects during molecular dynamics simulations of mechanical deformation (Ruhr-University Bochum)

2013

Dr.-Ing. M. Asgari: Pulsed Plasma Nitriding - Effect on Hydrogen Embrittlement and Hydrogen Adsorption and Diffusion (Norwegian University of Science and Technology NTNU, Trondheim, Norway)

Dr. rer. nat. S. G. Ayodele: Lattice Boltzmann modeling of advection-diffusion-reaction equations in non-equilibrium transport processes (RWTH Aachen)

Dr.-Ing. K. Davut: Relation between microstructure and mechanical properties of a low-alloyed TRIP steel (RWTH Aachen)

Dr.-Ing. R. D. Kamachali: Grain boundary motion in polycrystalline materials (Ruhr-Universität Bochum)

Dr. rer. nat. J. Klemm: Element resolved corrosion analysis of stainless steel-type glass forming steels and the correlation to their microstructure (Ruhr-Universität Bochum)

Dr.-Ing. C. Kords: On the role of dislocation transport in the constitutive description of crystal plasticity (RWTH Aachen)

Dr. rer. nat. R. Krieg: Untersuchungen zur Inhibition der Sauerstoffreduktion durch Zink-basierende Korrosionsproduktschichten (Ruhr-Universität Bochum)

Dr. rer. nat. J. C. Meier: Degradation phenomena and design principles for stable and active Pt/C fuel cell catalysts (Ruhr-Universität Bochum)

Dr. rer. nat. S. Nayak: Investigation of Electrochemical Oxygen Reduction on Semiconductor Surfaces by Attenuated Total Internal Reflection Infrared Spectroscopy (Ruhr-Universität Bochum)

Dr.-Ing. S. C. M.-F Reeh: Elastic and plastic properties of fcc Fe–Mn based alloys (RWTH Aachen)

Dr.-Ing. B. Salgin: Monitoring of the oxide-chemistry controlled surface ion mobility (Ruhr-Universität Bochum)

Dr. rer. nat. P. Schneider: Studie über die Anfangsstadien und die Aktivierungsprozesse der Phosphatierung auf aluminium- und siliziumhaltigen Oberflächen (Ruhr-Universität Bochum)

Dr.-Ing. D. Steinmetz: A constitutive model of twin nucleation and deformation twinning in High-Manganese Austenitic TWIP steels (RWTH Aachen)

Dr.-Ing. T. Takahashi: On the growth and mechanical properties of non-oxide perovskites and the spontaneous growth of soft metal nanowhiskers (RWTH Aachen)

Dr. rer. nat. G. K. Tirumalasetty: Mechanics in Steel through Microscopy (TU Delft, The Netherlands)

Dr. rer. nat. H. Zandbergen: Mechanics in Steel through Microscopy (TU Delft, The Netherlands)

2014

Dr. rer. nat. P. J. Bach: Lithiation and delithiation mechanisms of model anodes for lithium ion batteries using the example of Au thin films: Correlation of electrochemical and in-situ high energy X-ray diffraction characterization (Ruhr-Universität Bochum)

Dr. rer. nat. P. F. Beese-Vasbender: From Microbially Induced Corrosion to Bioelectrical Energy Conversion - Electrochemical Characterization of Sulfate-Reducing Bacteria and Methanogenic Archaea (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. W. Guo: Co-deformation of Amorphous CuZr/Nanocrystalline Cu Multilayers (Ruhr-Universität Bochum)

Dr. rer. nat. N. Hamidi Siboni: Molecular Dynamics Studies of Thermodynamical Consistency and Non-locality of Effective Temperature (RWTH Aachen)

Dr. rer. nat. D. Iqbal: Ultrathin Chemisorbed Polymer Coatings: Corrosion Protection and Nanostructuring of ZnO (Ruhr-Universität Bochum)

Dr.-Ing. M. I. Isik: Nucleation of Mo-rich Laves phase particles in 12% Cr steels (Ruhr-Universität Bochum)

Dr.-Ing. T. Jäpel: Feasibility study on local elastic strain measurements with an EBSD pattern cross correlation method in elastic-plastically deforming material (RWTH Aachen)

Dr.-Ing. J. Kahlen: Development of Models and Methods to Simulate Peptide-Assisted Nucleation and Growth of Calcium-Minerals (Mainz University)

Dr. rer. nat. S. Mandal: Dynamic correlations and confinement effects in glass forming hard sphere systems (RWTH Aachen)

Dr.-Ing. F. Moszner: Fe–Mn–Pd maraging steels for biodegradable implant applications (ETH Zurich, Switzerland)

Dr.-Ing. G. A. Nematollahi: Multiscale description of super-saturated ferrite in severely deformed pearlitic wires (Ruhr-Universität Bochum), with distinction “summa cum laude”

Dr.-Ing. K. G. Pradeep: Atomic scale investigation of clustering and nanocrystallization in FeSiNbB(Cu) soft magnetic amorphous alloys (RWTH Aachen), **with distinction “summa cum laude”**

Dr. rer. nat. L. Schemmann: The inheritance of different microstructures found after hot rolling on the properties of a completely annealed dual phase steel (RWTH Aachen)

Dr. rer. nat. A. K. Schuppert: Combinatorial screening of fuel cell catalysts for the oxygen reduction reaction (Ruhr-Universität Bochum), **with distinction “summa cum laude”**

Dr.-Ing. W. Song: Characterization and simulation of bainite transformation in high carbon bearing steel 100Cr6 (RWTH Aachen), **with distinction “summa cum laude”**

Dr. rer. nat. A. A. Topalov: Design and implementation of an automated electrochemical flow system coupled with mass spectrometry for investigation of the dissolution behavior of platinum (Ruhr-Universität Bochum), **with distinction “summa cum laude”**

Dr. mont. B. Völker: Investigation of interface properties of barrier metals on dielectric substrates. PhD Thesis, Department of Physical Metallurgy and Materials Testing (Montanuniversität Leoben, Austria), **with distinction “summa cum laude”**

Dr. mont. A. C. Wimmer: Plasticity and fatigue of miniaturized Cu structures (Montanuniversität Leoben, Austria), **with distinction “summa cum laude”**

Dr.-Ing. X. Wu: Structure-property-relations of cuticular photonic crystals evolved by different beetle groups (Insecta, Coleoptera) (RWTH Aachen)

Dr. X. Zhang: Structural transformations in Fe-C alloys: From atomistic simulations to a microscopic understanding (Ruhr-Universität Bochum)

2015

Dr.-Ing. C. Baldizzone: Degradation of Carbon-Supported Pt Bimetallic Nanoparticles (Ruhr-Universität Bochum), **with distinction “summa cum laude”**

Dr.-Ing. M. M. Belde: Designing ductile martensitic steel microstructures via localised austenite formation controlled by tailored chemical gradients (RWTH Aachen)

Dr. rer nat. S. T. Cheng: A density functional theory study on the oxidation behaviour of Mg and Mg-Zn alloys (Ruhr-Universität Bochum)

Dr.-Ing. M. Diehl: High Resolution Crystal Plasticity Simulations (RWTH Aachen), **with distinction “summa cum laude”**

Dr. rer. nat. A. Glensk: Anharmonic contributions to *ab initio* computed thermodynamic material properties (Universität Paderborn)

Dr. Phil. Y. Guo: The interactions between slip band, deformation twins and grain boundaries in commercial purity titanium (Oxford University, UK)

Dr.-Ing. S. Gupta: Micromechanical modeling of martensitic phase transformation in steels based on non-local crystal plasticity (Ruhr-Universität Bochum)

*Dr. rer. nat. C. Heinz*l: Correlation of structure and performance in high temperature polymer electrolyte membrane fuel cells (LMU Munich), **with distinction "summa cum laude"**

Dipl.-Ing. Dr. mont. Peter J. Imrich: TEM investigations on interactions of dislocations with boundaries (Montanuniversität Leoben, Austria), **with distinction "summa cum laude"**

Dr. rer. nat. S. Kenmoe: Ab Initio Study of the Low-Index Non-Polar Zinc Oxide Surfaces in Contact with Water: from Single Molecules to Multilayers (Ruhr-Universität Bochum)

Dr.-Ing. M. Kuzmina: Segregation driven phase transformation in medium Mn steel (RWTH Aachen), **with distinction "summa cum laude"**

Dr. rer. nat. M. Lange: The microstructural influence on high temperature corrosion in DMV617mod under coal-fired conditions (RWTH Aachen)

Dr. rer. nat. C. A. Laska: Development of a Scanning Flow Cell system with Dynamic Electrolyte Change for Fully Automated Parameter Screening (Ruhr-Universität Bochum)

Dr. rer. nat. Z. Pei: Theory-guided combinatorial materials design of ductile Mg-based alloys: employing *ab initio* and atomistic methods (RWTH Aachen)

Dr. rer. nat. S. Pengel: Anwendung eines Quantenkaskadenlasers in der zeitaufgelösten Laserabsorptionsspektroskopie zur kinetischen Untersuchung der elektrochemischen Sauerstoffreduktion an Germanium (Ruhr-Universität Bochum)

Dr.-Ing. F. Ram: The Kikuchi Bandlet Method (RWTH Aachen)

Dr. rer. nat. L. Rossrucker: Electrochemical dissolution characteristics of Zn, Mg, Al and ZnMg(Al) alloys (Ruhr-Universität Bochum)

Dr. rer. nat. T. Schwarz: On the nano-scale characterization of kesterite thin-films (RWTH Aachen), **with distinction "summa cum laude"**

Dr. rer. nat. D. Tytko: Thermal stability of AlN/CrN superlattice hard coatings (RWTH Aachen)

Dr. rer nat. A. Vimalanandan: Investigation of Redox-Responsive Coatings for Zinc Corrosion Protection (Ruhr-Universität Bochum)

Diploma Thesis

2013

Baron, C.: Mikrostrukturelle und mechanische Untersuchungen an legierten perlitischen Drähten (Hochschule Coburg)

Master Theses

2013

Cai, P.: Study of Dislocation-Twin Boundaries Interaction Using Discrete Dislocation Dynamics simulations (RWTH Aachen)

Li, X.: Microstructure and mechanical properties of Fe–Al–Ti–B alloys with addition of Mo and W (RWTH Aachen)

Morsdorf, L.: Nanocrystallization in soft-magnetic Fe-Si-B amorphous alloys / Nanokristallisation in amorphen weichmagnetischen Fe-Si-B-Legierungen (RWTH Aachen)

Nguyen, C.-D.: Structural interactions between solid-melt interfaces (Ruhr-Universität Bochum)

Stechmann, G.: Crystallographic and Electronic Characterization of Grain Boundaries in CdTe Thin Film Solar Cells (ENSCL Lille, France)

Tarzimoghadam, Z.: Investigation of mechanical properties, microstructures and plastic deformation of near-alpha Ti-Mo and Ti-Fe alloys (RWTH Aachen)

Wang, Z.: Residual stress measurements in TWIP steels by nano-indentation and delta EBSD (RWTH Aachen)

Witt, U.: Entwurf und Implementierung eines gestenbasierten Natural User Interface zu Werkstoffmodellierung (Universität Duisburg-Essen)

Yao, M.: Non-equiatomic FeMnNiCoCr high entropy alloys: microstructure, phase stability and mechanical behavior (RWTH Aachen)

2014

Archie, F. M. F.: Nanostructured High-Mn Steels by High Pressure Torsion: Microstructure-Mechanical Property Relations (RWTH Aachen)

Hu, Q.: Nanoscale tribocorrosion at model metal and metal oxide interfaces (Ruhr-Universität Bochum)

Krieger, W.: Fügen von Stahl und Aluminium bei Raumtemperatur (Ruhr-Universität Bochum)

Li, Z.: Optimization and application of Electron channelling contrast imaging (ECCI) technique under controlled diffraction conditions (cECCI) for investigation of dislocation in Ni-based superalloy (RWTH Aachen)

Pang, B.: Synthesis of photosensitive molecules and characterization of their adsorbates on Au(111) Surface (Ruhr-Universität Bochum)

Peng, Z.: Investigation of ruthenium effect on the formation of topologically close-packed phases in nickel based superalloys

Rechmann, J.: Oberflächenmodifizierung von Zink (Eisen) mit Ethinylphenothiazinen und Charakterisierung (Heinrich-Heine-Universität Düsseldorf)

Sheng, Z.: Characterization of the Microstructure and Mechanical Properties of Maraging Steels Produced by Laser Additive Manufacturing (RWTH Aachen)

Sözen, H. I.: Ab initio investigations on the energetics and kinetics of defects in Fe–Al alloy. (Ruhr-Universität Bochum)

Spies, M.: Influence of growth conditions on the opto-electronic properties, microstructure and chemistry of $Cu_2ZnSnSe_4$ thin-films (Heinrich-Heine-Universität, Düsseldorf)

Wan, D.: Electron Channeling Contrast Imaging (ECCI) Analysis on Deformed Aluminum (RWTH Aachen)

Wang D.: Crystal Plasticity Simulations on the Formation of Shear Bands. (RWTH Aachen)

2015

Afshar, M.: Experimental investigation of the co-deformation of Mg-matrix and LPSO precipitates across phase (RWTH Aachen)

Grabowski, M.: Implementation of atomic spin constraints in the density-functional theory package S/PHI/nX (Heinrich-Heine Universität Düsseldorf)

Gupta, A.: Precipitation Kinetics in Binary Alloys (Ruhr-Universität Bochum)

Müller, M.: Influence of solvated ions on hydrophobic interactions (Fachhochschule Südwestfalen)

Naikade, M.: Testing of a new software tool for the determination of the amount of recrystallized and recovered volume fraction and its application to different annealed aluminum alloys (RWTH Aachen)

Schwenzfeier, K.: Aggregation von Amphiphilen an der Wasser/Luft-Grenzfläche (Ruhr-Universität Bochum)

Sharma, L.: Implementation and comparison of different damage criteria in the framework of crystal plasticity (Ruhr-Universität Bochum)

Tecklenburg, S.: Electrochemical Attenuated Total Reflection Infrared Spectroscopic experiments at Hydrogen terminated Silicon single crystal surfaces (Ruhr-Universität Bochum)

Twiste, F.: Phase field modeling of oxide scale growth (Heinrich-Heine-Universität Düsseldorf)

Weikamp, M.: Instabilities during frictional sliding between strongly dissimilar materials (Heinrich-Heine-Universität Düsseldorf), **with top mark**

Bachelor Thesis

2013

Cox, K.: Elektrochemische Untersuchung von Eisen im Schwefelwasserstoff gesättigten Elektrolyten (Hochschule Niederrhein)

Grabowski, M., Entwicklung und Validierung DFT-basierter EAM-Potentiale (Heinrich-Heine-Universität Düsseldorf)

2014

Welk, D., Elastische Wechselwirkungen zwischen Punktdefekten im Superzellansatz: Modellrechnung in 1 - 2 Dimensionen (Heinrich-Heine-Universität Düsseldorf)

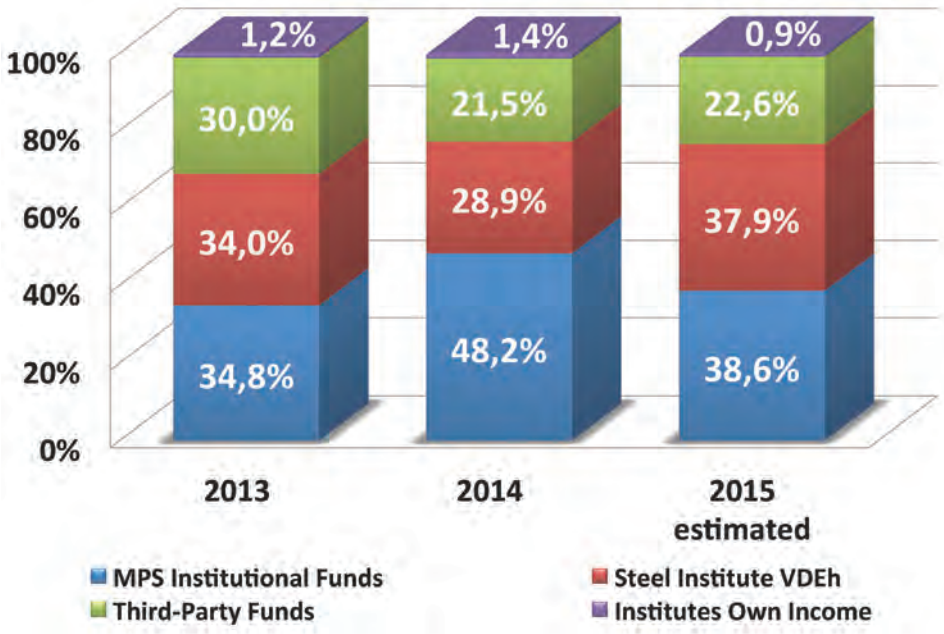
2015

Bottler, F., GPU simulation and visualization of microstructure evolution (Fachhochschule Jülich-Aachen-Köln)

Budget of the Institute

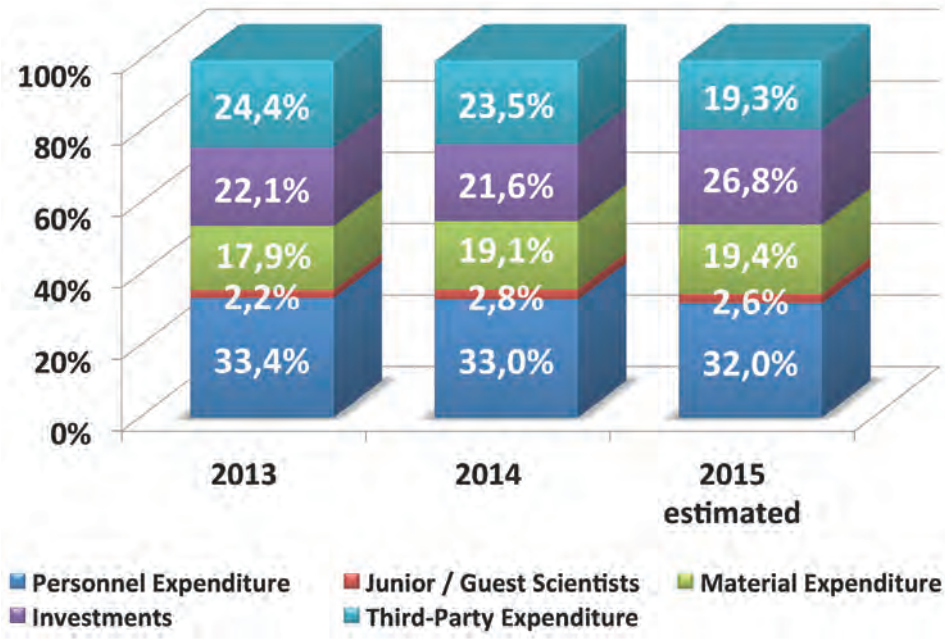
Revenue

(percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2015 data estimated)



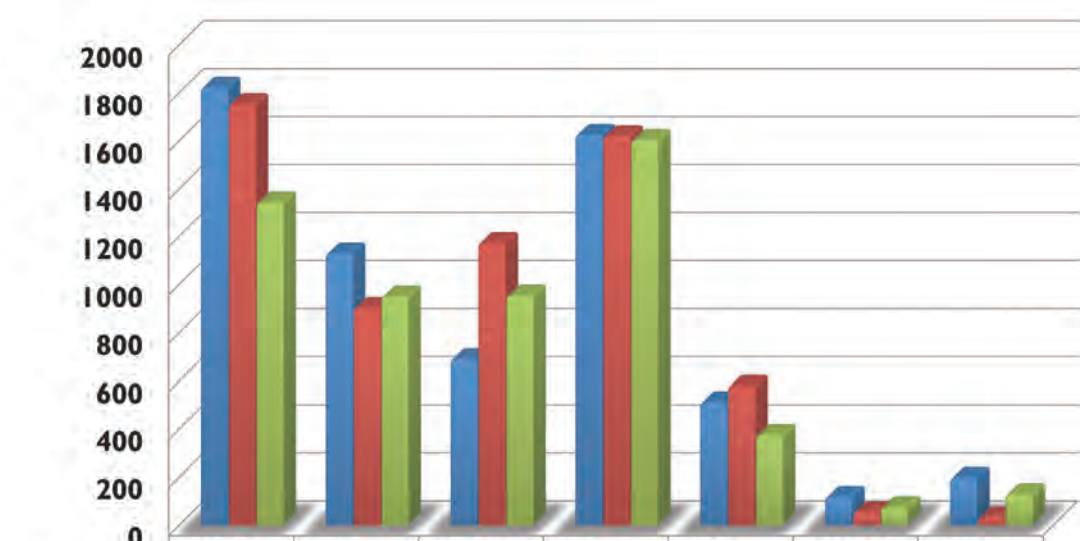
Expenditure

(percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2015 data estimated)



Third-Party Funds

(Contributions in 1,000 € to total revenue including personnel, material and investements, year 2015 data estimated)



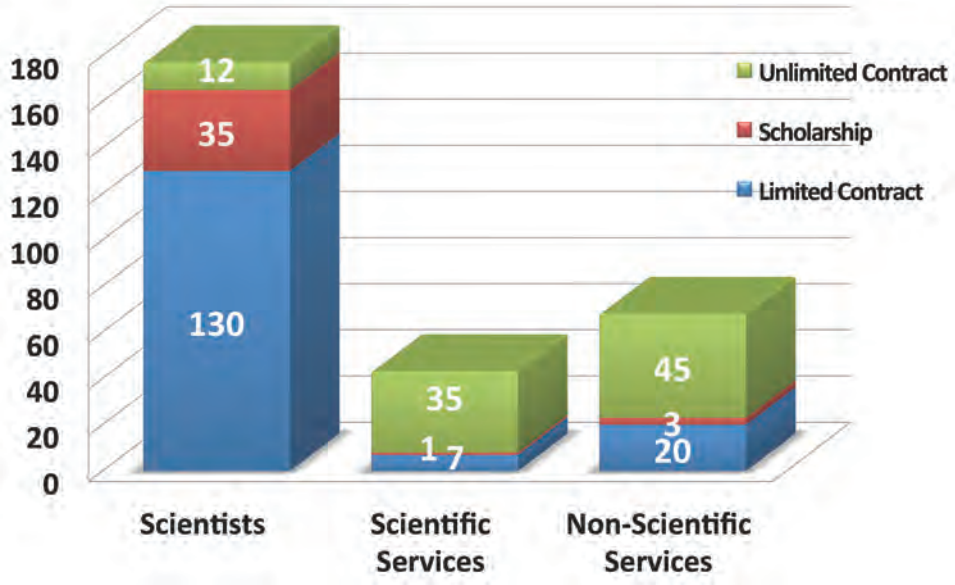
	DFG	EU/ RFCS	Federal	Industry	MPS	NRW	Others
2013	1818	1125	685	1621	507	114	193
2014	1749	899	1170	1615	575	51	29
2015 (est.)	1339	947	950	1599	371	71	126

DFG: German Science Foundation
EU: European Union
RFCS: Research Fund for Coal and Steel
Federal: BMBF & BMWi
BMBF: Federal Ministry of Science and Education
BMWi: Federal Ministry of Economics and Technology
Industry incl. Christian Doppler Society and MaxNet
MPS: Max Planck Society
NRW: State of North Rhine-Westphalia
Others: Diverse expenditure on material costs (e.g. Humboldt Foundation, Merkle Foundation)

Personnel Structure

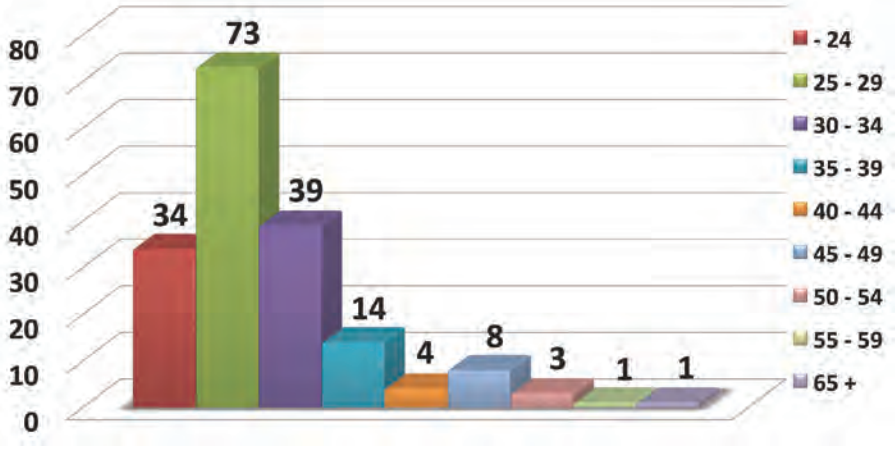
Number of Occupied Scientific / Non-Scientific Positions

(Absolute Numbers, July 2015)



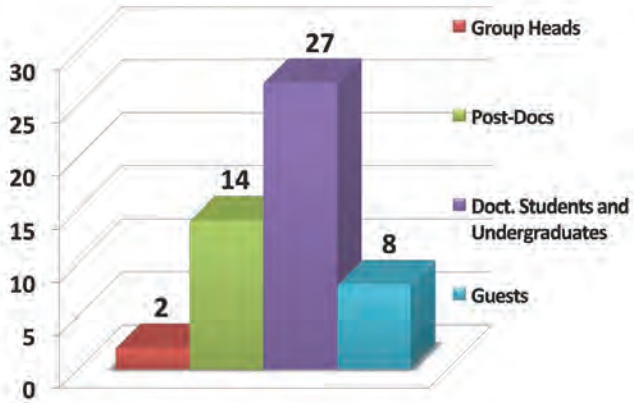
Age Distribution of Scientists

(Absolute numbers, July 2015)



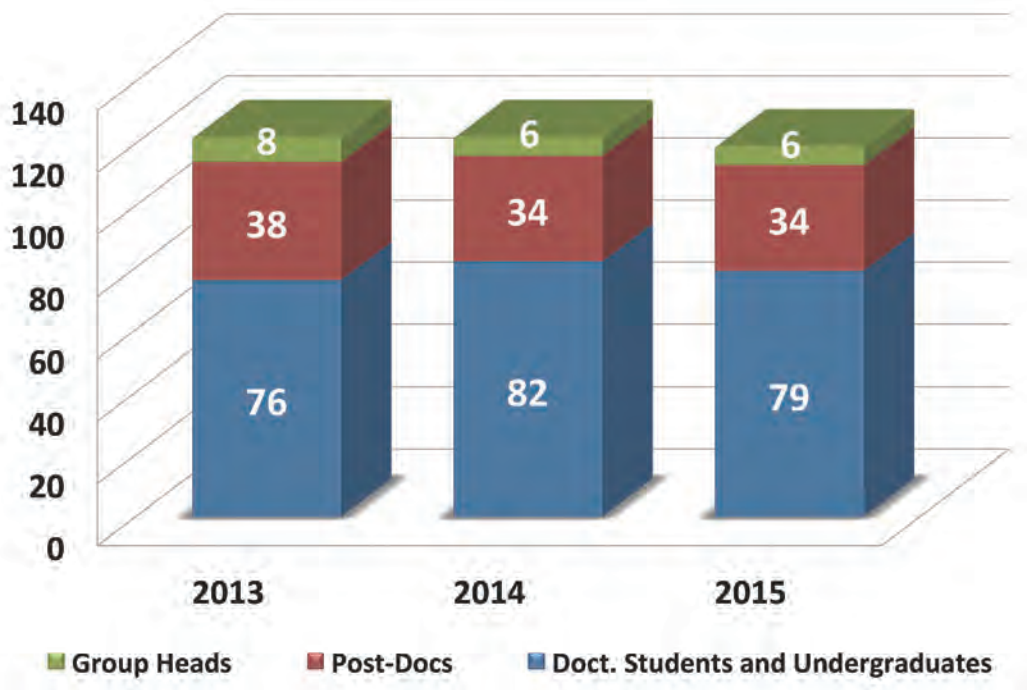
Female Scientists

(Absolute numbers, July 2015)

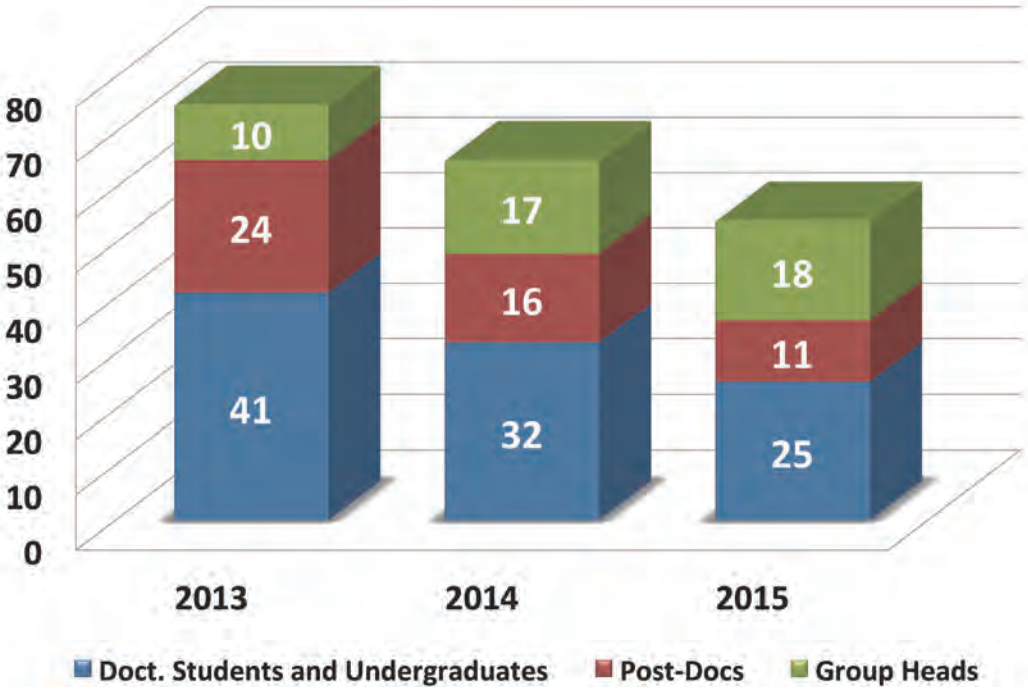


Number of Junior Scientists (Absolute numbers, year 2015 data estimated)

Financed via Third-Party Funds



Not Financed via Third-Party Funds



Scientists and their Home Countries

(Absolute numbers, July 2015)